

# Screening Level Ecological Risk Assessment for Area of Concern-4 (AOC-4)

# **Remedial Investigation/Feasibility Study**

Falcon Refinery Superfund Site Ingleside, San Patricio County, Texas EPA Identification No. TXD086278058

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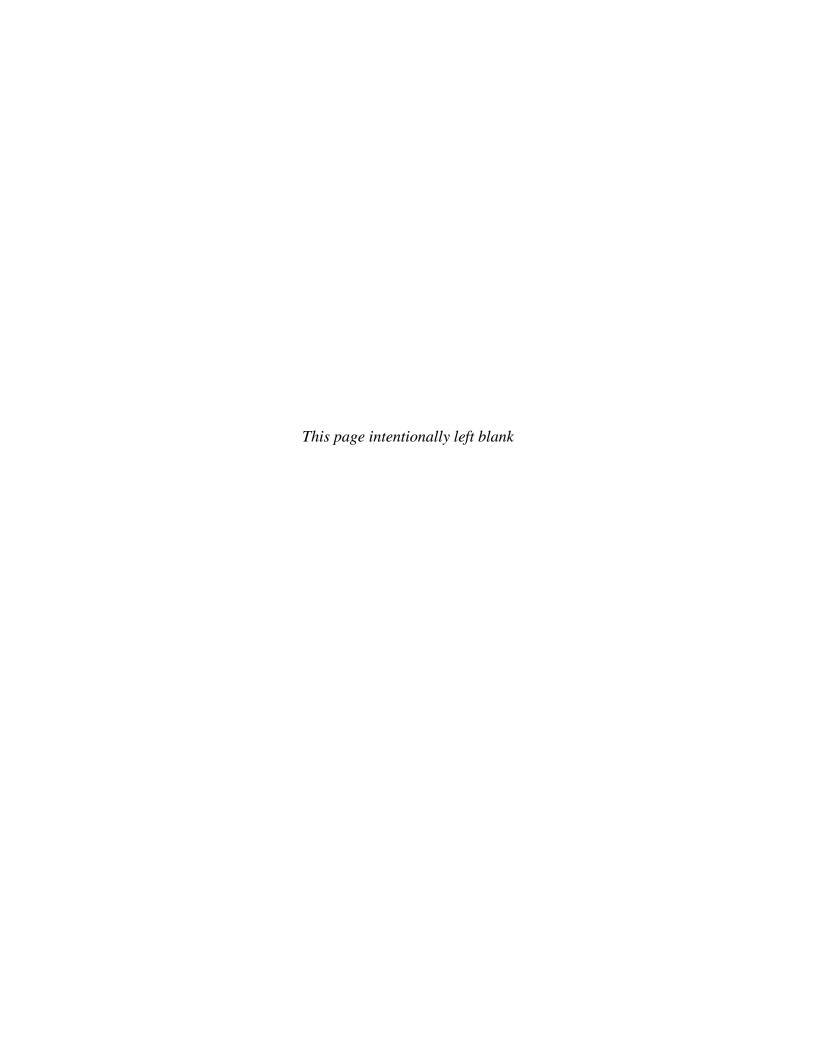
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#### LIST OF ACRONYMS AND ABBREVIATIONS

AOC Area of Concern

AST Above ground storage tank

BAF Bioaccumulation Factor BCF Bioconcentration Factors

BRAPF Baseline Risk Assessment Problem Formulation

BW Body weight

CHPPM U.S. Army Center for Health Promotion and Preventative Medicine

COPEC Chemicals of Potential Ecological Concern

CSM Conceptual Site Model

d Day

EA Engineering, Science, and Technology, Inc.

Eco-SSL Ecological Soil Screening Level

EPA U.S. Environmental Protection Agency

EPC Exposure Point Concentration ERA Ecological risk assessment

FI Food ingestion FM Farm-to-Market FS Feasibility Study

HMW High molecular weight

HQ Hazard Quotient

ICW Intracoastal Waterway

kg Kilogram

Lazarus Texas Refining I, LLC

LMW Low molecular weight

LOAEL Low Observed Adverse Effect Levels

mg/kg Milligrams per kilogram mg/L Milligrams per liter

ND Non-detect

NOAEL No Observed Adverse Effect Levels NORCO National Oil Recovery Corporation

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# LIST OF ACRONYMS AND ABBREVIATIONS (CONTINUED)

ORNL Oak Ridge National Laboratory

PAH Polynuclear aromatic hydrocarbon PRG Preliminary Remediation Goal PRP Potentially Responsible Party

RI Remedial Investigation

Site Falcon Refinery Superfund Site

SLERA Screening Level Ecological Risk Assessment

SQL Sample quantitation level

SVOC Semivolatile organic compound

TAL Target analyte list

TCEQ Texas Commission on Environmental Quality

TPWD Texas Parks and Wildlife Division

TRV Toxicity reference value

UCLM Upper confidence level of the mean

UF Uptake factor

UPL Upper prediction limit

USFWS U.S. Fish and Wildlife Service

VOC Volatile organic compound

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#### 1. INTRODUCTION

EA Engineering, Science, and Technology, Inc. (EA) has been authorized by the U.S. Environmental Protection Agency (EPA), under Remedial Action Contract Number EP-W-06-004, Task Order 0088-RICO-06MC, to conduct a Remedial Investigation/Feasibility Study (RI/FS) at the Falcon Refinery Superfund Site (Site). EPA's scope of work includes the preparation of a Screening Level Ecological Risk Assessment (SLERA) for the Site. EPA has requested that EA prepare a SLERA for the barge dock area (Area of Concern [AOC] 4) and the Intracoastal Waterway (ICW; aka AOC-5) separate from the remaining Site. This document provides the results of the SLERA for AOC-4. The SLERA for AOC-5 is completed as a second document.

#### 1.1 SITE BACKGROUND AND DESCRIPTION

The Site is located 1.7 miles southeast of State Highway 361 on Farm-to-Market (FM) 2725 at the north and south corners of the intersection of FM 2725 and Bishop Road near the City of Ingleside in San Patricio County, Texas (Figure 1). The Site occupies approximately 104 acres and consists of a refinery that operated intermittently. The refinery is currently inactive and has not produced hydrocarbon products in several years except for a crude oil storage operation being conducted by Superior Crude Gathering, Inc. When in operation the refinery had a capacity of 40,000 barrels per day and the primary products consisted of naphtha, jet fuel, kerosene, diesel, and fuel oil. The refinery also historically transferred and stored vinyl acetate, a substance not excluded under the petroleum exclusion.

The Site is divided into the North Site, South Site and current barge dock facility. There are pipelines that connect the North and South Sites with the current and former barge dock facilities. The North Site consisted of nine above ground storage tanks (ASTs), three truck loading racks, associated piping, and a transfer pump. The South Site consisted of the main operations of the refinery. This area had a control room, heaters, crude towers, coalesers, boilers, fire water tank, exchangers, cooling towers, desalters, exchangers, compressors, a lab, 24 ASTs, separator, clarifiers, and aeration pond (TRC 2013). The barge dock facility (AOC-4) is located on Redfish Bay (AOC-5) and was used to load and unload crude oil and refined hydrocarbons via pipelines that connect the dock to the North and South Sites.

The Site was proposed to the National Priorities List on 5 September 2002. The Potentially Responsible Party for the Site, National Oil Recovery Corporation (NORCO), entered into an "Administrative Order on Consent" with the EPA on 9 June 2004, to perform and finance the removal action and RI/FS for the Site.

In 2012, NORCO sold the former Falcon Refinery to Lazarus Texas Refining I, LLC (Lazarus), which operates the former refinery as a crude oil bulk storage and transfer facility. Lazarus is attempting to obtain a notice of no further action for the barge dock facility to obtain a "bridge

loan" until additional funding can be obtained (TRC 2013). Lazarus plans to further develop the Site through remedial actions and upgrades.

The Site has been divided into AOCs based upon former use and location (Figure 2). AOC-1 consists of the Former Operational Units and includes the entire North Site, and a drum disposal area and metal waste disposal area which are part of the South Site. AOC-2 includes areas of the refinery that were not used for operations or storage and have no record of releases. AOC-3 encompasses the wetlands immediately adjacent to the Site that are bordered by Bay Avenue, Bishop Road, and a dam on the upstream side; wetlands located between Bishop Road, Sunray Road, Bay Avenue, and residences along Thayer Avenue; and the wetlands between Sunray Road, residences along FM 2725, Gulf Marine Fabricators, Offshore Specialty Fabricators, and the outlet of the wetlands into Redfish Bay. Within AOC-3, there are one active and several abandoned pipelines that lead from the refinery to the barge dock facilities. During June 2006, the abandoned pipelines were cut, the contents of the pipelines were removed, and plates were welded on the pipelines. AOC-4 includes the barge docking facility. AOC-4 is approximately 1.6 acres and is located on Redfish Bay. The fenced facility, which is connected to the refinery by pipelines, is used to load and unload barges. Currently only crude oil passes through the docking facility. Historically, refined products were also loaded and unloaded. AOC-5 encompasses the sediments and surface water within the ICW adjacent to the barge dock facility. AOC-6 includes the neighborhood along Thayer Road, across from the refinery. AOC-7 includes the neighborhood along Bishop Road, across from the North Site.

# 1.2 SITE INVESTIGATIONS

Initial field sampling was conducted in 2007 in accordance with an EPA approved RI/FS Field Sampling Plan and Quality Assurance Plan for the former refinery, adjacent properties, and background sampling locations (TRC 2013). Analytical data obtained during the sampling was evaluated for ecological exposures, and results indicated that further sampling was necessary to adequately assess certain portions of the Site. EA conducted Phase II investigation activities in accordance with the Final Field Sampling Plan (EA 2013) and Quality Assurance Project Plan (EA 2012) under this Task Order in 2013. Surface soil and surface soil background data tables for AOC-4 are presented in Appendix A-1 and A-2, respectively.

# 1.3 AOC-4 BACKGROUND AND DESCRIPTION

AOC-4 is the current barge docking facility which occupies approximately 1.6 acres adjacent to the ICW. The fenced facility is connected to the refinery by pipelines and is used to load and unload barges. It was reported that only crude oil passed through the docking facility. However, refined products historically were loaded and unloaded at this docking facility. There have been no reported releases associated with this AOC. However, analytical results indicate that a release or releases have occurred. Although there is no indication from the boring cores that fill material is present at the Site, historical aerial photos show that the area generally consisted of wetlands in the 1950s. It is likely that the elevation of the Site was raised with fill material for its industrial purpose and also because of the potential for flooding and hurricanes in the area.

#### 2. ECOLOGICAL RISK ASSESSMENT

This section presents the SLERA conducted by EA for AOC-4 at the Site. The purpose of this assessment is to characterize and quantify potential environmental impacts from residual chemicals in soil at AOC-4 from Site activities. The assessment was conducted in accordance with EPA guidance for the RI/FS process; specifically the ecological risk assessment (ERA) was conducted in accordance with the process for ERAs outlined in the document *Ecological Risk Assessment Guidance for Superfund: Process for Designing and Conducting Ecological Risk Assessments* (EPA 1997), other relevant EPA guidance, as well as the Texas Commission on Environmental Quality (TCEQ) guidance *Conducting Ecological Risk Assessments at Remediation Sites in Texas* (TCEQ 2014a) and *Texas Surface Water Quality Standards* (TCEQ 2010).

The process for ERA outlined in EPA guidance includes eight steps (EPA 1997, 1998), and this document presents the first three steps of the ERA process (Figure 3). Steps 1 and 2 represent the SLERA. The SLERA uses highly precautionary assumptions regarding exposure and toxicity to develop a Conceptual Site Model (CSM) and identify Chemicals of Potential Ecological Concern (COPECs). The CSM defines complete and significant exposure pathways and identifies assessment and measurement endpoints. The screening level evaluation typically relies on chemical analytical data.

Step 3 of the SLERA process is the Baseline Risk Assessment Problem Formulation (BRAPF). The BRAPF draws from the risk evaluation performed in the SLERA to identify COPECs, exposure pathways, assessment endpoints, and risk questions requiring further consideration. The BRAPF often includes refinement of the screening level risk calculations through use of more realistic or more relevant exposure and toxicity data. The goal of the BRAPF is to provide a clear definition of the ecological risk problems for the Site. This problem formulation forms the basis for either further assessment or, in cases where sufficient data are available, risk management if necessary.

In the case of the Falcon Refinery Superfund Site, a SLERA and BRAPF refinement of risk calculations were performed at AOC-4. Section 2.1 presents the CSM and assessment endpoints. Section 2.2 discusses the data used in the SLERA and presents measurement endpoints for the screening level risk evaluation. Section 2.3 presents the SLERA results and conclusions. Section 2.4 presents the refined risk assessment and methodology and discusses the data and measurement endpoints used. The refined toxicity assessment is defined in Section 2.5, and the refined risk calculation is defined in Section 2.6. Results from the BRAPF for AOC-4 are presented in Section 2.7. The results for all measurement endpoints are combined in a qualitative weight of evidence approach to provide a preliminary risk characterization for each assessment endpoint. Uncertainties associated with the risk assessment are presented in Section 2.8, and results of the risk characterization are considered together in developing the conclusions for the Site which are presented in Section 3.0.

#### 2.1 SUMMARY OF DATA USED IN THE SLERA

Initial field sampling was conducted in 2007 in accordance with an EPA approved RI/FS Field Sampling Plan and Quality Assurance Plan for the former refinery, adjacent properties, and background sampling locations (TRC 2013). Analytical data obtained during the sampling was evaluated for ecological exposures, and results indicated that further sampling was necessary to adequately assess certain portions of the Site. Field activities conducted in 2013 as part of the Phase II Field Sampling Plan had objectives relating to this SLERA which included providing data to identify and delineate the extent of COPECs in environmental media, identify potential and complete exposure pathways, and provide data for completion of human health and ERAs as well as the feasibility study. Table 1 presents the samples collected in 2013 that were used in this risk assessment.

A total of six surface soil samples were collected from AOC-4 in 2013 as shown in Figure 4. For the purposes of the ERA, surface soil is defined as the top 0 to 6 inches below ground surface. This is considered the zone of greatest potential exposure for ecological receptors. The soil was analyzed for target analyte list (TAL) metals, polynuclear aromatic hydrocarbons (PAHs), semivolatile organic compounds (SVOCs), and volatile organic compounds (VOCs).

Investigation of soil for the Site included collection and analysis of samples from 10 locations representative of background conditions. These locations were selected to be beyond the suspected influence of the Falcon Refinery Site. Background data are evaluated in the BRAPF to aid in risk management decisions. Details regarding background sampling can be found in the Field Sampling Plan for the investigation effort (EA 2013).

# 2.1.1 Data Reduction and Summary Statistics

This section describes the approach that was followed to evaluate the available analytical data in the medium of concern (surface soil). The following list summarizes the approach:

- Analytical results with a "R" qualifier (indicating that the data were rejected during the validation process) were not used in the SLERA and BRAPF.
- Analytical results with a "U" or "UJ" qualifier indicate that the analyte was not detected
  at the sample quantitation level (SQL). These data were considered non-detects (NDs)
  and were retained in the data set. In the calculation of the 95 percent upper confidence
  limits of the mean (UCLMs), each ND was assigned a numerical value of one-half its
  SQL.
- Analytical results with a "J" qualifier indicate that the reported values were estimated
  because the analyte was detected at a concentration below the SQL or for other reasons.
  These data were considered detections and were retained in the data set at the measured
  concentration.

- Analytical results with "D", "K", or "L" qualifiers were considered detections and were retained in the data set at the measured concentration.
- Inorganic analytes with "B" or "BJ" qualifiers were retained in the data set at the measured concentration.
- Analytical results for organic analytes with a "B" qualifier (blank-related data) were treated as NDs.

In accordance with EPA (1989) guidance, the following steps were first used to summarize the chemical analytical data for the SLERA:

- Sample data were compared to blank (laboratory, equipment rinse, and field) concentration data. If the chemical concentration detected in a site-related sample was less than 10 times (for common laboratory chemicals) or 5 times (for all other compounds) the concentration detected in the corresponding blank sample, the sample was treated as a ND. The identification and validation of sampling or laboratory artifacts were performed prior to data summarization.
- The maximum concentration of a pair of duplicate or split samples (taken from the same location on the same date) if both parent and duplicate were detected, the maximum non-detect concentration if both parent and duplicate were non-detects, and the detected value if either parent or duplicate were detected, and the other non-detected were used to represent the concentration for that location.
- Frequency of detection was calculated as the number of samples in which the chemical was detected over the total number of samples analyzed.

There are a number of uncertainties associated with the chemical analytical data associated with sample coverage and study design. Uncertainties associated with the data used in the SLERA are discussed in Section 2.5.

# 2.2 ECOLOGICAL CONCEPTUAL SITE MODEL

As part of the CSM, potential sources of chemicals and exposure pathways are characterized for the Site (Figure 5). The model illustrates the pathways through which receptors may be exposed to sources of COPECs. Sources and exposure pathways are discussed further below.

# 2.2.1 Ecological Setting

The Falcon Refinery Superfund Site consists of a refinery that had the capacity of 40,000 barrels per day with the primary products consisting of naphtha, jet fuel, kerosene, diesel, and fuel oil. The refinery operated intermittently and is currently inactive. The Site encompasses approximately 104 acres in San Patricio County, Texas with portions of the Site (AOC-4 and

AOC-5) located along Redfish Bay in the ICW. The property includes piping that leads from the Site to dock facilities at Redfish Bay, where crude oil and hydrocarbons were historically and are currently being transferred between barges and storage tanks to adjacent properties. The current barge dock facility is fenced and contains several small structures to load and unload crude oil. There have been no reported spills or releases, and there are no visible indications of environmental impacts at the barge dock facility.

# 2.2.2 Vegetation and Physical Habitat

The barge dock facility (AOC-4) consists of approximately 1.6 acres. The barge dock facility is fenced, contains several small structures, and is comprised primarily of compacted silty sand and gravel. AOC-4 borders AOC-5 (evaluated separately) which includes the ICW; other than the ICW, no additional sensitive environmental areas exist within 500 feet of AOC-4.

Based on aerial photographs and direct observation during site visits, AOC-4 is mostly barren of vegetation with scattered patches of herbaceous vegetation interspersed among the roads and storage areas. Plant species consist primarily of disturbance-tolerant grasses and forbs. As such, AOC4 is expected to provide relatively poor, isolated habitat for wildlife.

Site visits have identified that soils at the Site are disturbed and compacted due to vehicle traffic and storage. Soil survey data (CSRL 2014) indicates that local soils consist of former dredged material, with some areas consisting of moderately alkaline massive clays while other areas consist of moderately alkaline fine sands. Based on this information and the soil boring at location MW-17, AOC-4 consists of moderately alkaline compacted silty sand and gravel. This substrate's compacted structure presents physical and nutritional challenges to colonization and establishment of plant and soil invertebrate communities. Given the proximity of the ICW and potential for flooding during hurricanes, salinity may play a natural role in limiting plant growth and diversity. Thus AOC-4 is likely to provide relatively poor habitat for plants and invertebrates.

Restoration of the Site to higher quality habitat faces challenges unrelated to chemical concentrations in soil. Although there are no restrictions or institutional control documenting that the property will remain industrial for future use, the Deed No. 615663 has a section called "Assumption of Obligations" and states that the "Falcon Refinery" has been designated by the EPA as a Superfund Site, and is subject to remediation and clean-up in connection with two (2) Administrative Orders On Consent. Existing soil is compacted and disturbed; should restoration occur at the Site, it would require major physical changes to the substrate such as mixing, addition of organic matter, or re-grading.

# 2.2.3 Threatened and Endangered Species

An important consideration in forming an ecological conceptual model is the presence of endangered, threatened, and rare species on the Site. As part of this assessment, the U.S. Fish and Wildlife Service (USFWS 2014a) and the Texas Parks and Wildlife Division (TPWD 2014a) program databases were searched for species that may utilize AOC-4 and the adjacent wetlands

and waterways. Two endangered and five federally and/or state listed threatened species may exist near the project area but would primarily utilize the aquatic habitat of AOC-5:

# **Endangered Species**

Whooping crane (*Grus americana*)—Federally Endangered, State Endangered Whooping cranes migrate through the area and are not residential. They typically feed in shallow water on fish, crustaceans, and other small marine animals, although they occasionally forage in fields (USFWS 2014b). Whooping cranes are not expected to utilize AOC-4, as none of these habitats are present.

<u>Eskimo curlew (Numenius borealis)</u>—Federally Endangered, State Endangered Eskimo curlew migrate from the Arctic tundra to South America and only temporality utilize grassland habitat in Texas (TPWD 2014b). Since AOC-4 has no grassland habitat, it is not expected that the Eskimo curlew will utilize the Site.

# **Threatened Species**

<u>Piping plover (Charadrius melodus)</u>—Federally Threatened, State Threatened Piping plovers are commonly found along sandy shorelines where they utilize the habitat for nesting and forage on small marine organisms (TPWD 2014c). They are not expected to use AOC-4 due to lack of suitable habitat.

# Sooty tern (Sterna fuscata)—State Threatened

The Sooty tern is a rare shorebird not commonly found along the east coast of Texas (TPWD 2014d). Due to their rarity and requirements for shore habitats and foraging grounds, Sooty terns are not expected to be found at AOC-4.

# Reddish egret (*Egretta rufescens*)—State Threatened

Reddish egrets are shorebirds that nest on the ground near bushes or on oyster shell beaches and they forage in brackish, marine, or freshwater habitats (TPWD 2014e). Reddish egrets are not expected to utilize AOC-4.

# Wood stork (Myctena americana)—State Threatened

Wood stork is a highly migratory species that utilizes shore habitat for foraging (TPWD 2014d). There have been no recent listings of wood stork in San Patricio County, and are therefore not expected to be present at AOC-4.

# White-face ibis (*Plegadis chihi*)—*State Threatened*

White-face ibis overwinters in warm climates and some are also permanent residents of the Texas east coast. They are most common in marshes, swamps, and riverine habitats with emergent vegetation (TPWD 2014 f). Since AOC-4 does not contain any suitable habitat, White-face ibis are not expected to utilize AOC-4.

Although it is not likely for any of these listed species to utilize AOC-4 due to the lack of habitat and adequate prey species, a more extensive analysis and biological survey would be needed to determine whether or not additional state listed species utilize the Site.

#### 2.2.4 Potential Source Areas

The primary source area is the barge docking facility. The property includes piping that leads from the Site to dock facilities at Redfish Bay, where crude oil and hydrocarbons were historically and are currently being transferred between barges and storage tanks to adjacent properties. There have been no reported releases associated with this AOC, however, analytical results indicated that a release or releases have occurred in the past. Based on the Site history, TAL metals, PAHs, SVOCs, and VOCs were analyzed in the soils at AOC-4.

# 2.2.5 Fate, Transport, and Media of Concern

A number of fate and transport pathways are expected to influence the transfer of COPECs between environmental media in the Site. Chemicals in surface soil at AOC-4 may have been transferred vertically to subsurface soil by leaching beyond the zone of exposure for ecological receptors, or horizontally to soil further from the source. Given the tendency for some of the COPECs at the Site (metals and PAHs) to bind to soil, horizontal transport is expected to be limited. The Site also consists of heavily compacted soils and has minimal changes in elevation.

The Site is at risk of flooding from hurricanes. Given the highly compact nature of the soil and the sea wall bordering Redfish Bay, it is unlikely that substantive amounts of COPECs in soil would migrate via storm runoff to the ICW during large storm events. The marine site AOC-5 is being evaluated separately.

It is important to note that transport pathways are dependent upon factors that influence the forms of chemicals in environmental media and their bioavailability. This is especially important for metals. Metals are present in nature in a wide range of chemical forms. Soluble forms of some metals are highly mobile in soil, sediment, and water, facilitating higher transport rates and making them more bioavailable, meaning that they are taken up more easily by plants and animals. Metals such as barium, copper, chromium, lead, nickel, vanadium, zinc, and others are more soluble in acidic or highly alkaline environments, and less soluble in circum-neutral or moderately alkaline environments. Soil surveys for the area around AOC-4 (CSRL 2014) indicate that soils tend to be moderately alkaline; therefore, many metals are expected to be less mobile and less bioavailable.

# 2.2.6 Identification of Media of Concern & Potential Receptors of Concern

Based on the above discussion of potential habitats, sources, and fate and transport, surface soil was considered the primary medium of concern (Figure 5). Potential receptors evaluated at AOC-4 in the SLERA for the Site include plants, soil invertebrates, amphibians and reptiles, birds, and small mammals. Potential ecological receptors are shown in the CSM (Figure 5).

# **Identification of Exposure Pathways**

Based on the ecological setting and media of concern discussed above, ecological receptors potentially present in AOC-4 include plants, terrestrial invertebrates, wildlife (birds and mammals), and reptiles and amphibians (Figure 5). Media of concern and ecological receptors are evaluated to determine potential exposure routes linking the two and to determine which pathways are complete and significant. The sections below identify the major routes of exposure and their applicability to each of these receptor groups.

#### **Terrestrial Plants and Invertebrates**

Terrestrial plants and invertebrates may be exposed to environmental media through direct contact. Plants may absorb chemicals from surface and subsurface soil via their roots. They may also absorb chemicals from air or airborne particles through their leaves, although the waxy surfaces of leaves limit this exposure. Terrestrial invertebrates may be exposed to chemicals in soil through direct contact and chemicals may be absorbed from soil through the skin. Because the most organic matter is found in the top 0 to 6 inches, plant and invertebrate exposures are expected to occur primarily in surface soil. Therefore, exposure pathways linking plants and soil invertebrates to surface soil are complete and therefore relevant for assessment.

# Wildlife (Birds, and Mammals)

The most significant exposure route for wildlife is ingestion of chemicals in contaminated media (EPA 2003a). Wildlife may ingest chemicals in environmental media by incidentally ingesting soil while grooming or foraging. As discussed above, chemicals may bioaccumulate in animal tissues. Therefore, wildlife may also ingest chemicals through the animals that they consume as food. Ingestion of chemicals in sediment, surface water, and/or food is considered a complete and potentially significant exposure pathway for wildlife at AOC-4.

Wildlife may be exposed to chemicals in air, sediment, or water via direct contact during foraging or burrowing. Most wildlife have protective outer coverings such as fur, feathers, or scales that prevent or limit the dermal absorption of chemicals from environmental media (CHPPM 2004). EPA guidance identifies that, in most cases, dermal exposures are likely to be less significant than exposures through ingestion and their evaluation involves considerable uncertainty (EPA 2003a, CHPPM 2004). Given that many metals demonstrate relatively low dermal absorption, this exposure route is considered complete but relatively insignificant for wildlife.

Inhalation is a potentially complete pathway for both terrestrial invertebrates and wildlife. These animals may inhale chemicals that have volatilized or that are adsorbed to airborne particulates. EPA guidance indicates that, in general, inhalation pathways are likely to be insignificant compared to ingestion pathways (EPA 2003a).

In summary, ingestion of chemicals in surface soil and food at AOC-4 are considered complete and significant exposure pathways for assessment in this SLERA.

# **Selection of Representative Receptors**

Ecological receptors that could possibly utilize the Site include plants, terrestrial invertebrates, and wildlife (reptiles, amphibians, birds, mammals). Selection of representative receptor species is based primarily on several factors: 1) the likelihood of a species to use the Site and the area immediately surrounding the Site, 2) the potential for exposure to site-related contaminants based on the feeding habits and life history of the organisms/guild represented by the receptor species, 3) the availability of life history and exposure information for the selected receptor species, and 4) the availability of toxicity information for the representative receptor species. Potential representative receptors were evaluated based on these criteria and based on the applicability of available toxicity benchmarks to plants, soil invertebrates, and wildlife at AOC-4. The receptors of concern (and representative receptor species) included in this SLERA are:

- Terrestrial plants (multiple species)
- Soil invertebrates (earthworm)
- Insectivorous birds (American robin)
- Insectivorous mammals (northern short-tailed shrew)
- Amphibians and reptiles (multiple species).

# **Terrestrial Plants**

Based on the general nature of available plant toxicity data, no specific plant species are selected for evaluation. Instead, the assessment evaluates the potential for adverse effects to herbaceous plant populations.

### **Terrestrial Invertebrates**

Earthworms were selected as the receptor species for evaluating the potential for adverse effects to soil invertebrates for several reasons. Earthworms have direct contact with soil and are sensitive to chemicals in soil, relative to other soil invertebrates. Furthermore, earthworms serve an important ecological role in the aeration of soils and cycling of nutrients and are an important food source for some soil invertebrate-eating species (e.g., robins and shrews). Lastly, toxicity data for earthworms are available in scientific literature.

### Wildlife

AOC-4 is an industrialized 0.5 acre site that is not expected to support a large diversity of terrestrial wildlife species. With the lack of suitable habitat and the presence of physical barriers for large predators, only smaller insectivorous species of birds and mammals were identified as potentially affected species.

While the risk assessments make conclusions concerning the potential for adverse effects to individual organisms, the objective is to be protective of the populations that may use AOC-4. However, few methods are available to extrapolate the potential for adverse effects from the

individual level to the population level. Therefore, it was assumed that if there is no potential for direct adverse effects to individual organisms, then it is also unlikely for there to be the potential for direct adverse effects to populations. Similarly, it was assumed that if there is the potential for adverse effects to individual organisms, then there is also the potential for adverse effects to populations. The following sections provide a summary of the avian and mammalian representative receptor species identified for evaluation.

# **Invertebrate-Eating Wildlife**

The American robin (*Turdus migratorius*) was selected as the invertebrate-eating avian species for evaluation, because a significant portion of its diet is comprised of earthworms and consequently, this species would have a higher rate of incidental ingestion of surface soil than an insect-eating bird species. The American robin also has an average home range of 1 to 2 acres (Young 1951, Pitts 1984).

The short-tailed shrew (*Blarina brevicauda*) was selected as the invertebrate-eating mammal species for evaluation because it feeds largely on soil invertebrates. Thus, it not only would be potentially exposed through prey items, but also would have a relatively high rate of incidental ingestion of soil while foraging. Furthermore, it has a small home range (0.07-4.4 acres) (EPA 1993) and thus could conceivably consume all of its diet from on-site.

In addition to the ingestion of chemicals in food items, the inadvertent ingestion of chemicals in surface soil was considered for the above species.

# **Amphibians and Reptiles**

The assessment of risks to amphibians and reptiles is limited by the lack of sufficient literature-based exposure and toxicity information. Also, there are currently no assessment methods for evaluating these receptors. The habitat at AOC-4 will most likely not support amphibian and reptile populations. Because potential risks to these receptors cannot be quantitatively dismissed, the amphibian and reptile receptor endpoints will be carried forward through the SLERA.

# 2.3 STEPS 1 & 2: SCREENING LEVEL ECOLOGICAL RISK ASSESSMENT

The first two steps of the 8-step ERA process (Figure 3) constitute the SLERA. The SLERA includes screening-level problem formulation, ecological effects evaluation, exposure estimate, and risk calculation. This section presents the SLERA for the Falcon Refinery Superfund Site and is organized into the following subsections:

- Screening-level problem formulation
- Summary of the SLERA results.

# 2.3.1 Screening Level Problem Formulation

The screening-level problem formulation includes development of a CSM and assessment and measurement endpoints. Assessment and measurement endpoints are identified for each representative receptor species evaluated at AOC-4 (Table 2). Measurement endpoints are measurable ecological characteristics that are related to the assessment endpoints (EPA 1997). The measurement endpoints are used to assess the potential for effects on the assessment endpoints through their comparison to screening level concentrations or toxicity values.

# 2.3.2 Measurement and Assessment Endpoints

EPA guidance stresses the importance of ecologically significant endpoints. As discussed by EPA, "Assessment endpoints are explicit expressions of the actual environmental value that is to be protected, operationally defined by an ecological entity and its attributes" (EPA 1998). Failure to select appropriate assessment and measurement endpoints can result in the inability to answer the risk questions central to an ERA. Several criteria are applicable for endpoint selection (Suter 1993; EPA 1998):

- 1. *Unambiguous Definition*—Assessment endpoints should indicate a subject and a characteristic of the subject (e.g., fish reproduction).
- 2. *Accessibility to Prediction and Measurement*—Assessment endpoints should be reliably predictable from measurements.
- 3. Susceptibility to the Hazardous Agent/Stressor—Susceptibility of an organism (plant or animal) results from the combination of potential for exposure and the sensitivity to the concentrations of contaminants or other stressors of concern.
- 4. **Biological Relevance**—Biological relevance of impacts to an individual organism is determined by the importance of the impact to higher levels of biological organization (e.g., populations or communities).
- 5. Social Relevance and Policy Goals—Assessment endpoints should be of value to decision-makers and the public. The assessment endpoints should represent effects that would warrant consideration of site remediation or alteration of project plans. Assessment endpoint selection should also include endpoints that may be mandated legally (e.g., protected species).

The ecological assessment endpoints applicable to this Site are discussed below:

• Protection of organisms exposed directly or indirectly to surface soil to ensure that COPECs in surface soil do not have unacceptable adverse effects on organism survival, growth, and reproduction, which may result in adverse effects to the community structure (e.g., diversity or biomass).

These assessment endpoints are general and are refined and revised for sample types warranting evaluation in the refined assessment conducted in Step 3.

The measurement endpoints are measurable ecological characteristics that are related to the assessment endpoints (EPA 1998). Because it is difficult to "measure" assessment endpoints, measurement endpoints were chosen that permit inference regarding the assessment endpoints described above. Measurement endpoints selected for this risk assessment are the following:

1. *Chemistry for Surface Soil*—The measurement of maximum COPEC concentrations in surface soil provides the means, when compared to conservative (based on chronic or no effects levels), ecotoxicological-based screening concentrations, for drawing inferences regarding the assessment endpoint for surface soil.

# 2.3.3 Identification of Chemicals of Potential Ecological Concern

COPECs are selected by comparison of maximum concentrations found in surface soil to EPA Region 3 and Region 4 ecological risk screening values, which coincide with TCEQ screening levels (TCEQ 2014a). Maximum concentrations in soil were compared to the lowest value obtained from the EPA Ecological Soil Screening Levels (Eco-SSLs), or EPA Region 4 screening values for soil which are found at the following links:

- Surface Soil—the lowest value obtained from the Eco-SSLs of available receptors from:
  - 1. EPA Eco-SSLs accessed at http://www.epa.gov/ecotox/ecossl
  - 2. Region 4 Ecological Screening Values, accessed at http://www.epa.gov/region4/superfund/programs/riskassess/ecolbul.html, or
  - 3. TCEQ—Table 3.4, accessed at <a href="http://www.tceq.texas.gov/assets/public/remediation/trrp/rg263-draft.pdf">http://www.tceq.texas.gov/assets/public/remediation/trrp/rg263-draft.pdf</a>

The criteria are presented in Table 3. Potential ecological risks associated with aluminum and iron in surface soils are identified based on pH. Aluminum and iron in surface soil can be identified as COPECs only at sites where the soil pH is less than 5.0 (EPA 2003a). The pH values for soils were not available for AOC-4, however soil pH is typically higher than 5.0, and considering the findings of CSRL (2014) that soils are moderately alkaline (pH > 7), neither metal was identified as a COPEC in surface soil samples during the initial screening.

# 2.4 SLERA RESULTS

Maximum exposure estimates were compared to media-specific screening levels and are shown in Table 4. The results of this risk calculation are used to identify COPECs. The SLERA risk calculation is performed by comparing the maximum exposure concentration to the screening level. When the screening level is greater than the maximum concentration, the potential for

adverse effects is considered unlikely. Because of the conservative nature of the SLERA, only chemicals with maximum concentrations less than the screening level can be removed from further examination. If the maximum concentration is equal to or greater than the screening level, or if a media-specific screening criterion is not available, the chemical is retained as a COPEC and examined further. Inclusion of these chemicals as COPECs does not necessarily indicate that they pose risks; it indicates that the chemicals cannot be definitively eliminated from further consideration. Essential nutrients, although detected in surface soil are not included in the list of COPECs. Essential nutrients include calcium, magnesium, sodium, and potassium.

The following chemicals exceed the surface soil screening value and were identified as COPECs. The Exposure Point Concentrations (EPCs) for these COPECs are shown in Table 4.

- Barium
- Cadmium
- Chromium
- Copper
- Lead
- Manganese
- Mercury
- Vanadium
- Zinc
- Total high molecular weight (HMW) PAHs.

The following SVOCs and VOCs were retained as COPECs due to lack of soil screening values. Risks from these detected chemicals cannot be determined and are typically discussed in the uncertainty evaluation of the ERA.

- Acetophenone
- Benzaldehyde
- Bis(2-ethylhexyl)phthalate
- Carbazole
- 2-Butanone
- Isopropylbenzene
- Trichlorofluoromethane
- Xylenes (m & p)
- Xylenes (o).

# 2.4.1 SLERA Conclusions

The SLERA identified COPECs in soil at AOC-4 that require further evaluation (Table 5). The results of the SLERA represent maximum estimates of risk, and are not necessarily representative of population-wide risks. Therefore, Step 3 of the ERA (the BRAPF) includes a refinement of risk estimates using more site-specific assumptions and information for AOC-4.

Risks from chemicals that do not have a screening value could not fully be evaluated and remain an uncertainty. Uncertainties associated with the SLERA are discussed in Section 2.8.

#### 2.5 ECOLOGICAL RISK ASSESSMENT REFINEMENT

The third step in the 8-step ERA process is required only for compounds for which the SLERA (Steps 1 and 2) indicates a need for further ecological risk evaluation. Consistent with ERA guidance (EPA 1997), highly conservative assumptions were used in the SLERA to provide an upper bound estimate of risk to ecological resources. Such an approach meets with the objectives of the SLERA, which are to screen out chemicals that do not have the potential to adversely affect ecological resources and to maintain chemicals that have potential to cause risks. These conservative assumptions are expected to over-estimate actual levels of risk to most ecological receptors. Consequently, some chemicals that pose negligible risk may be retained as COPEC at the outset of Step 3. The objective of the BRAPF is to determine the scope and goals of the baseline ERA by considering the results of the SLERA with additional site-specific information and alternate, more realistic assumptions in the estimates of risk. The results of this evaluation build upon the risk results presented in the SLERA and are intended to help in making scientific management decisions about the need for further investigation.

# 2.5.1 Refined Assessment and Measurement Endpoints

The following refined assessment endpoints were defined (Table 2) to reflect the potential impacts of the complete and significant exposure pathways at AOC-4 discussed above:

- Protection of terrestrial plant communities to ensure that COPEC in surface soils do not have unacceptable adverse effects on survival, growth, and reproduction of key plant species, which may result in adverse effects to the community structure.
- Protection of invertebrate communities to ensure that COPEC in surface soils do not have unacceptable adverse effects on survival, growth, and reproduction of key invertebrate species, which may result in adverse effects to the community structure, i.e., diversity or biomass.
- Protection of terrestrial wildlife to ensure that COPEC that have bioaccumulated in prey tissue do not have unacceptable adverse effects on survival, growth, and reproduction of representative receptor species.
- Protection of reptiles and amphibians to ensure that COPEC in soils do not have unacceptable adverse effects on survival, growth, and reproduction of key species.

Because assessment endpoints are often defined in terms of ecological characteristics that are difficult to measure (e.g., the health of a population or community), measurement endpoints are selected to provide a quantifiable means of characterizing risks. Measurement endpoints are quantifiable ecological characteristics that are related to each assessment endpoint (EPA 1989).

The following refined measurement endpoints were defined to draw inferences regarding the refined assessment endpoints.

- Protection of Terrestrial Plant Communities— The measurement of maximum COPEC concentrations in surface soil and the calculation of 95 percent UCLM COPEC concentrations in surface soil provide the means, when compared to relevant receptor-specific benchmarks, for drawing inferences regarding the first assessment endpoint above.
- 2. **Protection of Invertebrate Communities**—The measurement of maximum COPEC concentrations in soil and the calculation of 95 percent UCLM COPEC concentrations in soil provide the means, when compared to relevant receptor-specific benchmarks, for drawing inferences regarding the second assessment endpoint above.
- 3. **Protection of Terrestrial Wildlife**—The measurement of maximum COPEC concentrations in soil and the calculation of 95 percent UCLM COPEC concentrations in soil provide the means to model wildlife doses, which can be compared to relevant receptor-specific benchmarks, to draw inferences regarding the fifth assessment endpoint above.
- 4. *Protection of Reptiles and Amphibians*—The assessment of risks to amphibians and reptiles is limited by the lack of sufficient literature-based exposure and toxicity information. Also, there are currently no assessment methods for evaluating these receptors.

# **Plants and Invertebrates**

The measurement endpoints for plants and soil invertebrates include comparison of EPCs to benchmarks called toxicity reference values (TRVs) protective of exposures to soil. Potential risks to plants and soil invertebrates were evaluated by comparing EPCs in soil to TRVs for these media. TRVs represent the threshold above which effects are expected and below which no effect is expected. Conservative benchmarks have been selected to ensure that all chemicals that may pose a risk are accurately identified. Comparisons were initially made using maximum EPCs as a precautionary initial screen. Comparisons were then refined using mean and point-by-point concentrations as EPCs. As defined in EPA guidance (EPA 1997), the ratio of a chemical's concentration to its TRV is called a Hazard Quotient (HQ). HQs greater than or equal to 1.0 indicate a potential for unacceptable risk, while HQs less than 1.0 indicate no potential for unacceptable risk. Results of comparisons will be interpreted in light of the anticipated environmental chemistry of site media and spatial relationships that may affect comparison results and relevance.

Exposure estimates are not developed for amphibians or reptiles, because a quantitative measurement endpoint for this ecological resource cannot be identified. Literature and database resources were examined for exposure and toxicity information that could be used to

quantitatively evaluate risks to amphibians and reptiles. Despite searches of the EPA ECOTOX database, Canadian-based Reptile and Amphibian Toxicology Literature database, and other various literature sources, inadequate data are available for a quantitative evaluation. Therefore, the potentials for risks to amphibians and reptiles will be maintained as an uncertainty throughout this ERA (see Section 2.8: Uncertainties).

# Wildlife

For wildlife, measurement endpoints are based on the results of food web models that predict the dose of chemicals ingested by wildlife. These doses will be compared to TRVs for wildlife. The first measurement endpoint evaluated will be a comparison of doses based on maximum EPCs to no-effects TRVs. Refinement of the models will be conducted using 95 percent UCLM EPCs. As discussed above, HQs greater than or equal to 1.0 indicate a potential for unacceptable risk, while HQs less than 1.0 indicate no potential for unacceptable risk. Results of comparisons will be interpreted in light of factors that include the anticipated environmental chemistry of site media and spatial relationships that may affect comparison results and relevance. More detailed presentation of measurement endpoints is provided in Table 2.

# 2.5.2 Refined Exposure Assessment

Many of the measurement endpoints identified in Section 2.2 rely on exposure estimation using chemical analytical data. In some cases, chemical concentrations are used as the exposure estimate, and the calculated 95 percent UCLM concentrations are identified as EPCs for comparison to benchmarks. In other cases, chemical concentrations are the EPC inputs for food web models that estimate exposures as ingested doses. The exposure assessment identifies the models and input parameters that were used in benchmark comparisons and food web dose modeling. These parameters include identification of exposure point concentrations, food web model assumptions, and literature-based uptake factors. These are discussed on a receptor-by-receptor basis.

# **Exposure Point Concentrations**

EPCs are the COPEC concentrations that a receptor is assumed to be exposed to within AOC-4. Two separate EPCs were used in the ERA (Table 5). The initial measurement endpoint for each receptor consists of a screening level comparison of the maximum case scenario exposure estimate to no-effects benchmarks. Therefore, the maximum concentrations detected in onsite media were used as the EPC in exposure estimation. The maximum EPC is a realistic estimate of hot-spot exposures to organisms that may spend their entire lives in a small area. However, use of the maximum EPCs for assessment of some organisms is conservative and is likely to over-estimate risks because it assumes that individual organisms spend 100 percent of their time inhabiting and feeding from the most contaminated sample location at the Site.

Additional measurement endpoints were evaluated based on 95 percent UCLM concentrations found in onsite soils. Given the small area of AOC-4, high confidence was attributed to the

relevance of using 95 percent UCLMs as EPCs. The 95 percent UCLM is a more realistic and yet still conservative value for consideration of the Site-wide populations and exposures for mobile receptors, because it assumes an upper-bound estimate of the average exposure across the Site. The 95 percent UCLM concentration of a chemical within a given sample data grouping was calculated with the EPA statistical software package ProUCL Version 4.0 following EPA guidance (EPA 2002b, 2007a). ProUCL was used for calculating the 95 percent UCLMs in this risk assessment, as this program allows the user to calculate distribution-specific UCLMs, as well as UCLMs for data that do not exhibit a specific distribution (Appendix C). If the calculated 95 percent UCLM exceeded the maximum detected concentration, then the maximum concentration was used as the EPC. Where the 95 percent UCLM could not be calculated because of low-detection frequencies, the maximum was used in its place. This creates uncertainties that are discussed further in Section 8; however, it is consistent with the methods utilized in ProUCL Version 4.0.

# **Exposure Modeling for Lower Trophic Level Wildlife**

The measurement endpoints for terrestrial plants and soil invertebrates at AOC-4 include comparison of EPCs to TRVs protective of exposures to environmental media. The use of EPCs to represent exposures for these organisms is discussed further below (Tables 6 to 16).

**Terrestrial Plants**—Chemical concentrations measured in the soil of the Site were used to evaluate the potential for adverse effects to terrestrial plants. Consistent with EPA guidance (EPA 1997), the maximum detected concentration was used as the initial EPC in comparisons against benchmarks protective of plants. In addition, the chemical concentrations at each sample location were used as sample-specific EPCs in comparisons to benchmarks (Table 8); the results of these sample-specific comparisons were used to calculate site-wide frequencies of exceedance. Finally, a conservative estimate of the 95 percent UCLM concentration was evaluated as an EPC in comparisons to indicate the potential for population-wide impacts.

**Terrestrial Invertebrates**—Chemical concentrations measured in the soil at AOC-4 were used to evaluate the potential for adverse effects to terrestrial soil invertebrates. Consistent with EPA guidance (EPA 1997), the maximum detected concentration was used as the initial EPC in comparisons against benchmarks protective of soil invertebrates (Table 8). In addition, the chemical concentrations at each sample location were used as sample-specific EPCs in comparisons to benchmarks; the results of these sample-specific comparisons were used to calculate site-wide frequencies of exceedance. Finally, a conservative estimate of the 95 percent UCLM concentration was evaluated as an EPC in comparisons to indicate the potential for population-wide impacts.

# **Exposure Modeling for Higher Trophic Level Wildlife**

Food web modeling was used to derive the dose-based exposure estimates for wildlife. This section presents the methods used to quantify the potential exposure of wildlife to chemicals via the ingestion of food and surface soil. The methods are based on equations presented in EPA

(1993) and Sample et al. (1996). The equations and exposure parameters discussed below are consistent with EPA (1997) guidance and standard risk assessment practice.

Chemicals in the exposure media for each receptor were evaluated in the exposure models. Table 6 provides uptake factors for invertebrates used in the exposure models. Table 7 provides a summary of exposure parameters for the avian and mammalian representative receptor species identified for evaluation, and food web models are presented in Appendix B.

It should be noted that, in general, conservative assumptions were used in the food web models. The objective of the models is to provide an upper bound risk estimate. Accordingly, in almost all cases, actual risks are likely to be overestimated by the models. Uncertainties associated with conservative assumptions and other exposure estimation factors are discussed in Section 2.8.

Two separate EPCs were used in food web dose modeling. The initial measurement endpoint for each bird and mammal receptor consists of a screening level comparison of the maximum case scenario exposure estimate to No Observed Adverse Effect Levels (NOAELs) benchmarks. Therefore, the maximum concentration detected in on-site media was used as the EPC in exposure estimation for this endpoint. Use of the maximum is highly conservative and is likely to over-estimate risks because it assumes that wildlife spend 100 percent of their time inhabiting and feeding from the most contaminated sample location at the Site.

Therefore, food web modeling for the other wildlife measurement endpoints was based on the 95 percent UCLM concentration in the exposure media. The 95 percent UCLM is a more realistic value for consideration of the Site-wide population, because it assumes an average exposure across the Site. As discussed above, the 95 percent UCLM concentration of a chemical within a given sample data grouping was calculated as the 95 percent UCLM derived by the EPA statistical software package ProUCL Version 4.0. Where the 95 percent UCLM could not be calculated because of low detection frequencies, the maximum was used in its stead.

# **Ingestion of Chemicals From Abiotic Media**

Wildlife at AOC-4 may ingest soil while foraging or grooming. Therefore, food web models account for incidental ingestion of soil.

The following equation was used to calculate the dose of chemical wildlife would obtain from the ingestion of soil (Dose<sub>soil</sub>, milligram per kilogram [mg/kg]):

$$Dose_{soil} = Soil * C_{soil}$$

Where:

Dose<sub>soil</sub> = Amount of chemical ingested per day from soil (mg/kg-day)

Soil = Soil ingestion rate (kilograms soil per kilogram body weight per day [kg/kg-

day])

 $C_{soil}$  = Chemical concentration in surface soil (mg/kg).

Percent soil ingestion values taken from the scientific literature for the terrestrial wildlife species of concern were multiplied by the food ingestion rates (FI) for these species to estimate soil ingestion rates. A summary of the percent soil ingestion rates and food ingestion rates taken from the scientific literature is presented in Table 7.

# **Ingestion of Chemicals From Food**

Food item (soil invertebrates) concentrations were developed using Bioaccumulation Factors (BAFs)/Bioconcentration Factors (BCFs). In general, values were selected from defensible, compilation- and consensus-based sources or sources which include validated models (i.e., Sample et al. 1998a; Beyer and Stafford 1993; ORNL 2009) instead of values from single studies. First preference was given to regression equations derived from paired field- or laboratory-based measurements. Second preference was given to ratio-derived BAFs developed based on paired data of tissue concentrations compared to media concentrations, unless validation studies showed these to be preferable to regressions. Examples of regression and ratio BAF development can be found in Sample et al. (1998b). Third preference was given to modeled equilibrium partitioning-derived BAFs based on physical or chemical characteristics. If no values could be identified, a BAF or BCF of 1 was selected.

The following equation was used to calculate the dose of chemicals that a terrestrial wildlife species could obtain from the ingestion of food (Dose food/prey, mg/kg-day):

$$Dose_{food/prey} = FI * C_{food/prey}$$

Where:

FI = Food ingestion rate (kg/kg-day)

 $C_{\text{food/prev}}$  = Estimated maximum concentration of chemical in food (mg/kg).

A summary of the FI used in the SLERA for each of the terrestrial wildlife species selected for evaluation is presented in Table 7. The following section discusses the equations used to estimate chemical concentrations within each food group ( $C_{invert}$ ).

# **EPCs in Soil Invertebrates**

Concentrations were derived from literature-based uptake factors (UF) for uptake in earthworms (Table 6). When literature-based uptake factors for soil invertebrates were not available for the detected chemicals, tissue concentrations were derived using a default BAF of 1. Dry weight tissue concentration was calculated by multiplying the dry weight soil times the uptake factor or,

where a regression was used, by entering the dry weight soil concentration into the equation. The 95 percent UCLM case scenario tissue concentrations were calculated using the 95 percent UCLM dry weight soil concentration. Where conversion to wet weight values was required, soil invertebrates were considered to contain 75 percent moisture as a default (CHPPM 2004).

$$C_{benthos} = C_{soil} * UF$$

Where:

 $C_{soil}$  = Concentration of COPEC in soil (mg/kg);

UF = Uptake factor for chemicals in sediment (unit less).

# **Total Chemical Ingestion**

The total dietary exposure doses (Dose<sub>total</sub>, mg/kg body weight [bw]-day [d]) for small insectivorous birds (American robin) and insectivorous mammals (northern short-tailed shrew) for the evaluated COPEC were determined using the following equation.

$$Dose_{total} = Dose_{food +} Dose_{soil}$$

Where:

Dose food = Amount of chemical ingested per day from food (prey) (mg/kg bw-d);

Dose soil = Amount of chemical ingested per day from soil (mg/kg bw-d).

The total dietary intakes are compared to dietary toxicity values to determine if adverse effects are likely to occur to insectivorous wildlife from the ingestion of COPEC in food and soil.

# 2.6 REFINED TOXICITY ASSESSMENT

This section derives toxicity values for use in evaluating exposure estimates for each representative receptor reference values for evaluation. The TRVs represent concentrations or doses of the chemicals that are protective of the ecological receptors being evaluated. TRVs are compared to EPCs or estimated doses to evaluate each chemical's potential for adverse effects on the receptor in question. The following sections summarize TRVs for each indicator species or community identified for evaluation.

# 2.6.1 Overview of Bioavailability and Toxicity

The toxicity of chemicals is related to their bioavailability. Organic compounds may form complexes or compounds that bind them to soil and make them chemically inaccessible to ecological receptors. Alternatively, these elements and compounds may be present in forms that are easily dissolved and absorbed, or in forms that tend to bind to biological tissues. It is these

forms of easily absorbed chemicals that are most toxic. Most TRVs are based on forms of chemicals that are readily bioavailable.

# **Metals**

For metals, bioavailability is governed largely by formation of metallic compounds, binding to the soil matrix, and speciation. The compounds and bonds formed by metals are determined by reduction and oxidation (redox) reactions, by the dominant pH in soil and sediment, and by the presence of organic carbon. Toxicological benchmarks such as those provided in EPA Eco-SSLs are developed based on moderately bioavailable forms of metals; these benchmarks may overestimate toxicity for less bioavailable forms, or underestimate toxicity for more bioavailable forms. Acidity increases the bioavailability of many cationic metals, such as barium, chromium, copper, lead, vanadium, and zinc, which may become more soluble at pH below 5. Soil surveys for the area around AOC-4 (CSRL 2014) indicate that soils tend to be moderately alkaline; therefore, many metals are expected to be less mobile and less bioavailable. Some metals, such as aluminum, may also form complexes with iron oxides and hydroxides; this makes these metals less bioavailable and less mobile. The effect of acidity on other metals is complex; arsenic, for example may form compounds that are less bioavailable under acidic conditions; however, it may also become more bioavailable if arsenic bound to iron hydroxide compounds is released (Bodek et al. 1988).

Redox conditions and pH also determine the speciation of metals. Some metals may exist in different valence states or chemical forms that demonstrate different toxicity and bioavailability. For example, arsenic can be found in nature as As III or As V, with higher toxicity and mobility typically exhibited by As III (EPA 2005a).

# **Organic Compounds**

For organic compounds, the primary factors determining persistence, mobility, and fate are: (1) degradation, (2) volatilization, and (3) binding to soil. PAHs may degrade over time, resulting in lower concentrations.

Another factor affecting SVOCs (particularly low molecular weight [LMW] PAHs) and VOCs is volatilization. Concentrations of these chemicals may decrease in soil over time due to transfer to and dispersion in the air. Volatilization may be an important factor in eliminating them from soil. Expected contributions of these chemicals to air pathways are insignificant.

Perhaps the most important factor affecting fate of organic compounds in soil is their affinity for binding to fine grained soils and organic matter. Many organic compounds, including PAHs, are hydrophobic and will bind tightly to these soil particles. This decreases the mobility of these compounds, preventing them from dissolving in the water column. However, while the hydrophobicity of these organic compounds may decrease solubility, it may also increase their uptake into the tissues of biota and the potential for bioaccumulation. Hydrophobic compounds may bioaccumulate and biomagnify in fats and lipids within fish, invertebrates, or wildlife (EPA

2000). Soils at the Site tend to consist of fine sands with a low percentage of organic matter; therefore, binding to soil is not expected to be a significant factor affecting bioavailability of organics.

# 2.6.2 Plant TRVs for Exposure to Soil

To assess the potential for chemicals to adversely affect terrestrial plants, soil concentrations were compared to soil TRVs protective of plants (Table 8) (EPA 2005 a-h; EPA 2006; EPA 2007 b-g). TRVs from studies by Efroymson et al. (1997a) were established at a level associated with a 20 percent reduction in growth or other measured toxicological endpoints. This level is consistent with other screening level benchmarks for SLERA and the current regulatory approach. Because few toxicity values have been developed for organic chemicals, surrogate organic chemical TRVs were used for the evaluation of potential adverse effects to plants, as applicable; surrogates are identified in Table 8.

# 2.6.3 Soil Invertebrate TRVs for Exposure to Soil

To assess the potential for inorganic and organic chemicals to adversely affect soil invertebrates, soil concentrations were compared to TRVs protective of soil invertebrates (Table 8) (Efroymson et al. 1997b; EPA 2005 a-h; EPA 2007 b-g). TRVs protective of worms were used to assess the potential for inorganic and organic chemicals to adversely affect worms (Efroymson et al. 1997b). TRVs from studies by Efroymson et al. (1997b) were established at a level associated with a 20 percent mortality or other measured toxicological endpoint for earthworms. This level is consistent with other screening level benchmarks for SLERA and the current regulatory approach. Because few toxicity values have been developed for organic chemicals, surrogate organic chemical TRVs were used for the evaluation of potential adverse effects to soil invertebrates, as applicable (Table 8).

# 2.6.4 Wildlife TRVs

Chemicals identified as having the potential to adversely affect wildlife species were evaluated using dose-based toxicological benchmarks. Two types of benchmarks were used, each corresponding to a different level of ecological impacts for birds (Table 9) and mammals (Table 10). First, modeled doses were compared to dose-based NOAELs. NOAELs are doses that have been shown to cause no adverse impacts in test species. The NOAELs used in this ERA were derived from studies by Hill (1979), EPA Eco-SSLs (EPA 2005a-h, 2006, 2007b-g, 2008), and by Oak Ridge National Laboratory (Sample et al. 1996). The Oak Ridge National Laboratory NOAELs were generally derived based upon measurements of survival, growth, or reproduction in the laboratory. Values from EPA Eco-SSLs were derived through statistical analyses of results from multiple toxicological studies with multiple endpoints. Because NOAELs are conservative and highly protective, they were used as TRVs in this ERA.

The second set of benchmarks utilized was Lowest Observed Adverse Effects Levels (LOAELs). These are the lowest concentrations at which adverse effects are observed on individual test

organisms. The severity of effects considered "low level" varies based on the study from which LOAELs are derived; in general, they correspond to minor changes in growth or reproduction. LOAELs are useful because there is considerable uncertainty associated with NOAELs. Because NOAELs are associated with no effects in a test study, it is uncertain whether they are close to or far below the threshold value at which effects would first be observed. LOAELs thus serve to bound the range of NOAELs, and the threshold of toxic effects is considered to lie between the NOAEL and the LOAEL. Therefore, LOAELs were also utilized as TRVs. In some cases, LOAELs were available from studies by Oak Ridge National Laboratory (Sample et al. 1996). When LOAELs were not available from this source or exceeded NOAELs from EPA Eco-SSL sources, the data provided in EPA Eco-SSL documents was used to derive LOAELs. In all cases, the geometric mean of the bounded LOAELs for growth and reproduction was calculated; this approach is similar to that used for derivation of many Eco-SSL NOAELs.

In general, chemical exposures and toxicity were evaluated on a chemical-by-chemical basis. However, combined effects were evaluated for PAHs. EPA studies show that the PAHs can be grouped into HMW and LMW groups and concentrations summed for comparison to benchmarks (EPA 2007f). Toxicity evaluation using summed PAH concentrations is performed for invertebrates, birds, and mammals throughout the ERA.

TRVs could not be found for certain chemicals due to a lack of available information in the scientific literature. The uncertainty associated with the lack of TRVs is discussed in Section 2.8.

# 2.7 REFINED RISK CALCULATION

To calculate a refined estimate of risks, refined estimates of exposure are compared to receptor-specific TRVs. Risk calculation is performed by dividing EPCs by TRVs. As defined in EPA guidance (EPA 1997), the ratio of a chemical's concentration to its TRV is called an HQ. HQs greater than or equal to 1.0 indicate a potential for unacceptable risk, while HQs less than 1.0 indicate no potential for unacceptable risk. Results of comparisons will be interpreted in light of factors that include the anticipated environmental chemistry of site media and spatial relationships that may affect comparison results and relevance.

#### 2.7.1 Refined Risk Characterization

The purpose of the risk characterization is to draw conclusions regarding the potential for risks to each assessment endpoint/representative receptor. This is done using a qualitative weight of evidence approach in which results for each measurement endpoint are considered as lines of evidence. In general, lines of evidence that provide results based on site-specific data applicable at the population level are given the greatest weight. Per EPA guidance (EPA 1997), the focus of the ERA is to protect the ecological values at the Site-wide population or community level except where threatened or endangered species are concerned.

# 2.7.2 Comparisons to Receptor-Based TRVs

Receptor-specific COPEC for the Site were identified through the comparison of receptor-specific exposure estimates to TRVs. As presented in Section 2.5, TRVs were selected from the literature. Consistent with ERA guidance (EPA 1997), the models used to quantify the potential exposure to higher trophic level organisms were designed to estimate an upper bound potential for adverse effects to the selected representative receptor species. Therefore, exceedance of a TRV indicates the potential for adverse effects, but does not indicate that an adverse effect is occurring from the chemical (Tannenbaum et al. 2003).

The refinement of the risk calculation compares exposure estimates of the COPECs identified in the first phase to TRVs for each representative receptor species. For plant and soil invertebrates, the maximum detected chemical concentrations in soil are used as exposure estimates respectively.

LOAELs are a valuable indicator of risk because they provide an upper bound to NOAELs. Exceeding a NOAEL-based TRV does not necessarily indicate a risk, because NOAELs, by definition, correspond to no effects and may not be the highest concentration at which no effects occur. LOAELs provide a clear indication of potential effects and a potential for risk; therefore, comparisons to LOAEL-based TRVs provide an important tool for ERA. Comparisons focus on 95 percent UCLM case scenario exposure estimates because they are the most relevant estimates for mobile wildlife populations.

It is important to note that the quality of the TRV can influence the HQ. With metals, for instance, one must consider the bioavailable form of the metal from which the TRV is generated and the bioavailable/toxic form of the metal that is most likely present onsite. Additionally, other literature TRVs are available and may generate different HQs. Uncertainties associated with the selection and use of TRVs are discussed in Section 2.8.

TRVs are not available for all COPECs and, therefore, there is uncertainty associated with the lack of toxicity information for some COPECs. Chemicals that lacked TRVs or had exposure estimates that equaled or exceeded TRVs were considered a COPEC (with the exception of essential nutrients). Those chemicals that had exposure estimates below TRVs (HQs less than 1.0) were removed from further consideration.

# 2.7.3 Additional Factors for Consideration at AOC-4

Additional lines of evidence were considered when creating the qualitative weight of evidence approach for this SLERA. For each receptor, the following characteristics were factored into the risk characterization:

- Evaluation of site-specific factors affecting chemical bioavailability and toxicity by examining pH and soil characteristics as they may affect relevance of toxicity benchmarks;
- Habitat quality and area use examined in light of representative receptor habitat requirements and habitat use patterns;
- Factors affecting future land use and changes to site substrates;
- Frequency of detection, exceedance, and spatial distribution;
- Comparison to background concentrations.

# **Background Data**

Background data are not used to eliminate COPECs from consideration in this SLERA. However, per EPA guidance, cleanup does not focus on COPECs with concentrations that are consistent with regional background (EPA 2002). Therefore, background data specific to the project are used as comparison criteria as part of a weight of evidence approach to inform risk management. The upper prediction limits (UPLs) were calculated for background data using ProUCL (Version 4.0) and compared to the maximum detected concentration (Table 17, Appendix C).

Background concentrations were only available for metals (Appendix A-2). The following COPECs demonstrated a maximum detected concentration that exceeded the 95% UPL background concentration:

- Cadmium
- Copper
- Mercury
- Vanadium.

The following COPECs did not have a maximum detected concentration that exceeded the 95% UPL background concentration:

- Barium
- Chromium
- Lead
- Manganese
- Zinc.

These comparisons to background are discussed as a factor relevant to risk management at the end of the risk characterization for each receptor.

# 2.8 REFINEMENT AND PROBLEM FORMULATION

The results of comparisons performed for the SLERA refinement for AOC-4 are presented in Tables 11 through 17.

#### 2.8.1 Terrestrial Plants

The conceptual model for AOC-4 soil identifies protection of terrestrial plant survival, growth, and reproduction from impacts of COPECs in soil as an assessment endpoint. The following measurement endpoints were evaluated as indicators of risk to terrestrial plants (Table 11):

- Comparison of the chemical concentrations to benchmarks protective of plants including
  - o Comparison using maximum EPCs and
  - o Comparison of 95 percent UCLM EPCs.

Comparison of maximum concentrations to benchmarks is typically given the most weight in the weight of evidence approach because it is the most precautionary indicator of risks at specific locations (i.e. hotspots). However, due to the small size and nature of the disturbed habitat at AOC-4, comparison of the 95 percent UCLM concentrations to benchmarks had the strongest weight of evidence as an indicator of population-wide risks in this refinement of the SLERA.

# **Measurement Endpoint 1: Comparison of Maximum Soil Concentrations to TRVs Protective of Plants**

The first measurement endpoint evaluated was the screening-level comparison of maximum chemical concentrations in soil to literature-based TRVs protective of plants. When maximum EPCs of COPECs were compared to TRVs, concentrations of six metals (barium, chromium, manganese, mercury, vanadium, and zinc) exceed TRVs protective of plants grown in soil (Table 11).

# **Measurement Endpoint 2: Comparison of 95 Percent UCLM Soil Concentrations to TRVs Protective of Plants**

Comparison of 95 percent UCLM chemical concentrations in soil to plant TRVs was considered as a second measurement endpoint. Chromium did not have a calculated 95 percent UCLM, so the maximum concentration was utilized as the 95 percent UCLM. When the 95 percent UCLM EPCs were compared to TRVs, an HQ greater than 1.0 remained for barium, chromium, mercury, vanadium, and zinc (Table 11). Several chemicals did not have NOAEL-based TRVs available and the uncertainty associated with the lack of TRVs is discussed in Section 2.8.

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#### Additional Factors Relevant to Risk Characterization for Plants

A number of site-specific factors are relevant to interpretation of results of chemical comparisons and overall risk characterization for terrestrial plants. Additional factors were evaluated relevant to barium, chromium, mercury, vanadium, and zinc, the chemicals for which 95 percent UCLM exceed TRVs. Evaluation of the factors identified in Section 2.7.3, include the following:

- **Site-specific bioavailability and toxicity**—Soil surveys for the area around AOC-4 (CSRL 2014) indicate that soils tend to be moderately alkaline. Barium, chromium, vanadium, and zinc all demonstrate lower toxicity in moderately alkaline soils. Benchmarks for plants are derived from studies focused on moderately to highly bioavailable concentrations of metals. Therefore, toxicity associated with these metals is likely to be over-estimated.
- **Habitat quality**—As discussed in the CSM, soils at the Site consist of compacted silty sands in an environment periodically subjected to inundation in saline water. Compacted sand provides a poor substrate for plant growth, and saline environments limit plant diversity to species highly tolerant of free metal ions. As such, factors other than elevated concentrations of metals are likely to limit plant establishment and growth, and species diversity at the Site.
- **Future land use**—Based on the Site setting, future land use is likely to remain industrial. Should attempts be made to restore vegetative communities, major physical changes to the Site's substrates would be required to mitigate the effects of compaction, salinity, and low organic matter content. These changes would likely pose a much greater influence on plant growth and reproduction than the elevated metal concentrations identified at the Site.
- Frequency of detection and spatial distribution—For barium, mercury, vanadium, and zinc, risks are driven by a single high concentration at SO4-01 (809 mg/kg barium, 1.5 mg/kg for mercury, 21.3 mg/kg for vanadium, and 560 mg/kg for zinc) compared to the plant NOAEL of 500, 0.3, 2.0, and 160 mg/kg, respectively. These concentrations are at least two times higher than the next closest value. Because these exceedances are limited to a single location, risks to the populations of plants at the Site are low. Chromium exceeded the plant TRV by 2 to 17 times in all 6 samples; however, 4 of the detected concentrations were estimated below the laboratory reporting limits and a 95 percent ULCM could not be calculated.
- **Background concentrations**—AOC-4 maximum detected concentrations of barium, chromium, and zinc did not exceed the 95% UPL background concentrations, and therefore unlikely to warrant consideration in risk management

#### **Risk Characterization for Terrestrial Plants**

When 95 percent UCLM are compared to TRVs protective of terrestrial plants, barium, chromium, mercury, vanadium, and zinc are found in exceedance. However, a number of factors identify that the potential for risk from these metals is low for AOC-4. Specifically, metal bioavailability and toxicity are likely over-estimated; site habitats are subject to non-chemical factors that already limit plant growth and diversity, and would require extensive alteration to support higher quality habitat; and exceedances are limited in spatial distribution. Moreover, three of the five metals are consistent with background concentrations and would not warrant risk management.

#### 2.8.2 Soil Invertebrates

As part of the BRAPF, refined risk calculation and evaluation of qualitative lines of evidence were evaluated to characterize risks to soil invertebrates from COPEC in soil. The following measurement endpoints were evaluated as indicators of risk to benthic organisms.

- Comparison of the chemical concentrations to benchmarks protective of soil invertebrates, presented in Table 12, including
  - o Comparison using maximum EPCs and
  - o Comparison of 95 percent UCLM EPCs.

Comparison of maximum concentrations to benchmarks is typically given the most weight in the weight of evidence approach because it is the most precautionary indicator of risks at specific locations (i.e. hotspots). However, due to the small size and nature of the disturbed habitat at AOC-4, comparison of the 95 percent UCLM concentrations to benchmarks had the strongest weight of evidence as an indicator of population-wide risks.

### **Measurement Endpoint 1: Comparison of Maximum Chemical Concentrations to Soil Invertebrate TRVs**

The first measurement endpoint evaluated was the comparison of maximum EPCs in surface soil to literature-based benchmarks protective of soil invertebrates. The NOAEL-based TRVs selected were chosen to provide a highly conservative estimate of the potential for risk. When maximum EPCs of COPEC were compared to NOAEL-based TRVs, four metal concentrations exceeded TRVs for soil invertebrates (barium, chromium, mercury, and zinc) and had an HQ greater than or equal to 1.0. Results for this measurement endpoint indicate that there is a potential for risk from these chemicals, although this measurement endpoint is highly precautionary because it assumes maximum exposure. Several chemicals did not have NOAEL-based TRVs available and the uncertainty associated with the lack of TRVs is discussed in Section 2.8.

## Measurement Endpoint 2: Comparison of 95 Percent UCLM Chemical Concentrations to Soil Invertebrate NOAEL-Based TRVs

The second measurement endpoint evaluated was the comparison of 95 percent UCLM EPCs in soil to literature-based benchmarks protective of soil invertebrates. Only barium, mercury, and zinc had a calculated 95 percent UCLM, whereas the maximum concentration had to be used for chromium due to the guidelines outlined in Section 2.4. When the 95 percent UCLM EPCs of barium, mercury, and zinc were compared to TRVs, an HQ greater than 1.0 remained.

#### Additional Factors Relevant to Risk Characterization for Soil Invertebrates

A number of site-specific factors are relevant to interpretation of results of chemical comparisons and overall risk characterization for soil invertebrates. Additional factors were evaluated relevant to barium, chromium, mercury, and zinc, the chemicals for which 95 percent UCLM exceed TRVs. Evaluation of the factors identified in Section 2.7.3, include the following:

- **Site-specific bioavailability and toxicity**—Soil surveys for the area around AOC-4 (CSRL 2014) indicate that soils tend to be moderately alkaline. Barium, chromium, and zinc all demonstrate lower toxicity in moderately alkaline soils. Benchmarks for soil invertebrates are derived from studies focused on moderately to highly bioavailable concentrations of metals. Therefore, toxicity associated with these metals is likely to be over-estimated.
- Habitat quality—As discussed in the CSM, soils at the Site consist of compacted silty sands in an environment periodically subjected to inundation in saline water. Compacted sand provides a poor habitat for more sensitive soil invertebrates such as worms as do saline environments. This limits soil invertebrate diversity to species highly tolerant of free metal ions and compacted substrates. As such, factors other than elevated concentrations of metals are likely to limit soil invertebrate diversity and abundance at the Site.
- **Future land use**—Based on the Site setting, future land use is likely to remain industrial. Should attempts be made to restore native communities, major physical changes to the Site's substrates would be required to mitigate the effects of compaction, salinity, and low organic matter content. These changes would likely pose a much greater influence on soil invertebrate communities than the elevated metal concentrations identified at the Site.
- Frequency of detection and spatial distribution—For barium, mercury, and zinc, risks are driven by a single high concentration at SO4-01 (809 mg/kg barium, 1.5 mg/kg for mercury, and 560 mg/kg for zinc) compared to the soil invertebrate NOAEL of 330, 0.1, and 120 mg/kg, respectively. These concentrations are at least two times higher than the next closest value. Because these exceedances are limited

to a single location, risks to the populations of soil invertebrates at the Site are low. Chromium exceeded the soil invertebrate TRV by 5 to 44 times in all 6 samples.

• **Background concentrations**—AOC-4 maximum detected concentrations of barium, chromium, and zinc did not exceed the 95% UPL background concentrations, and therefore unlikely to warrant consideration in risk management

#### **Risk Characterization for Soil Invertebrates**

When 95 percent UCLM are compared to TRVs protective of terrestrial plants, barium, chromium, mercury, and zinc are found in exceedance. However, a number of factors modify concern for the potential for risk from these metals for AOC-4. In specific, metal bioavailability and toxicity are likely over-estimated; site habitats are subject to non-chemical factors that already limit soil invertebrate abundance and diversity, and would require extensive alteration to support higher quality habitat; and exceedances for some chemicals are limited in spatial distribution. Moreover, three of the four metals are consistent with background concentrations and would not warrant risk management.

#### 2.8.3 Terrestrial Avian Wildlife

The conceptual model for the Site identifies protection of the survival, growth, and reproduction of birds from impacts of COPECs in soil and food as an assessment endpoint. The conceptual model identified representative receptors from the insectivore feeding guild (American robin) for assessment. The following measurement endpoints were evaluated as indicators of risk to birds:

- Screening level comparison of maximum case scenario doses ingested through the food web to NOAEL and LOAEL-based benchmarks protective of birds
- Comparison of 95 percent UCLM case scenario doses ingested through the food web to NOAEL and LOAEL-based benchmarks protective of birds.

### Measurement Endpoint 1: Comparison of Maximum Case Scenario Modeled Doses to NOAEL and LOAEL Benchmarks Protective of Birds

The HQ for each chemical is calculated based on the comparison of the dose from maximum concentrations in soil to the NOAEL and the LOAEL (dose modeling presented in Appendix B). Dose modeling and comparisons to NOAEL-based literature TRVs using maximum EPCs identified six metals (barium, cadmium, copper, lead, vanadium, and zinc) as having an HQ equaling or exceeding 1.0 for insectivorous birds (Table 13).

Dose modeling and comparisons to LOAEL-based literature TRVs using maximum EPCs identified three metals as having an HQ equaling or exceeding 1.0 for insectivorous birds (barium, vanadium, and zinc) (Table 13).

## Measurement Endpoint 2: Comparison of 95 Percent UCLM Case Scenario Modeled Doses to NOAEL and LOAEL Benchmarks Protective of Birds

The second measurement endpoint evaluated the comparison of ingested doses for birds based on 95 percent UCLM EPCs in soil to NOAEL and LOAEL and literature-based TRVs protective of birds. Only barium, lead, vanadium, and zinc had a calculated 95 percent UCLM, whereas the maximum concentrations had to be used for cadmium due to low frequency of detection. When the 95 percent UCLM EPCs were compared to NOAELs, an HQ greater than 1.0 remained for barium, lead, vanadium and zinc for insectivorous birds (Table 14). When compared of LOAELs, vanadium and zinc continued to have an HQ greater than 1.0 for insectivorous birds (Table 14).

#### Additional Factors Relevant to Risk Characterization for Avian Wildlife

A number of site-specific factors are relevant to interpretation of results of chemical comparisons and overall risk characterization for avian wildlife. Additional factors were evaluated relevant to vanadium and zinc, the chemicals for which 95 percent UCLM exceed TRVs. Evaluation of the factors identified in Section 2.7.3, include the following:

- **Site-specific bioavailability and toxicity**—Soil surveys for the area around AOC-4 (CSRL 2014) indicate that soils tend to be moderately alkaline. Vanadium and zinc demonstrate lower bioavailability and toxicity in moderately alkaline soils. Uptake factors and benchmarks for birds are derived from studies focused on moderately to highly bioavailable concentrations of metals. Therefore, bioavailability and toxicity associated with these metals is likely to be over-estimated.
- **Habitat quality**—As discussed in the CSM, the Site provides poor quality habitat for wildlife, with little vegetation and few resources to support prey items such as soil invertebrates. The American robin has an average home range of 1 to 2 acres, and with the small size of AOC-4 and lack of suitable habitat for soil invertebrates, the robin is likely to forage outside of Site, and AOC-4 is likely to provide habitat for a very small population of birds.
- **Future land use**—Based on the Site setting, future land use is likely to remain industrial. Should attempts be made to restore higher quality habitat, major physical changes to the Site's substrates would be required that would greatly alter exposure concentrations.
- Frequency of detection and spatial distribution—Vanadium concentrations exceeded LOAELs in all six samples. Zinc concentrations exceeded LOAELs at three of the six sample locations by a factor of 1 to 4.

 Background concentrations—The AOC-4 maximum detected concentration of zinc did not exceed the 95% UPL background concentrations, and is therefore unlikely to warrant consideration in risk management.

#### Risk Characterization for Avian Wildlife

When 95 percent UCLM are compared to NOAELs protective of avian receptors, barium, lead, vanadium, and zinc are found in exceedance. When 95 percent UCLM are compared to LOAELs protective of avian receptors, vanadium and zinc are found in exceedance. However, a number of factors identify that the potential for risk from these metals is minimal for AOC-4. In specific, metal bioavailability and toxicity is likely over-estimated; site habitats are subject to non-chemical factors that limit their use by birds as a resource, and would require extensive alteration to support higher quality habitat; and exceedances are limited in spatial distribution. Moreover, concentrations of one of the two metals identified are consistent with background concentrations and would not warrant risk management.

#### 2.8.4 Terrestrial Mammalian Wildlife

The conceptual model for the Site identifies protection of the survival, growth, and reproduction of mammals from impacts of COPECs in soil and food as an assessment endpoint. The conceptual model identified representative receptors from the insectivore feeding guild (shrew) for assessment. The following measurement endpoints were evaluated as indicators of risk to mammals:

- Screening level comparison of maximum case scenario doses ingested through the food web to NOAEL and LOAEL-based benchmarks protective of mammals
- Comparison of 95 percent UCLM case scenario doses ingested through the food web to NOAEL and LOAEL-based benchmarks protective of mammals.

## Measurement Endpoint 1: Comparison of Maximum Case Scenario Modeled Doses to NOAEL and LOAEL Benchmarks Protective of Mammals

The HQ for each chemical is calculated based on the comparison of the dose from maximum concentrations in soil to the NOAEL and LOAEL (dose modeling is presented in Appendix B). Dose modeling and comparisons to NOAEL-based literature TRVs using maximum EPCs identified two chemicals (cadmium and zinc) as having an HQ equaling or exceeding 1.0 (Table 15).

Dose modeling and comparisons to LOAEL-based literature TRVs using maximum EPCs identified no COPECs as having an HQ equaling or exceeding 1.0 (Table 15).

## Measurement Endpoint 2: Comparison of 95 Percent UCLM Case Scenario Modeled Doses to NOAEL Benchmarks Protective of Mammals

The second measurement endpoint evaluated the comparison of ingested doses for mammals based on 95 percent UCLM EPCs to NOAEL and LOAEL-based TRVs. The HQ for each chemical is calculated based on the comparison of the dose from 95 percent UCLM concentrations in soil to the NOAEL and LOAEL. Zinc had a calculated 95 percent UCLM, whereas the maximum concentration was used for the cadmium due to low frequency of detection. An HQ greater than 1.0 remained for zinc during the comparisons of the 95 percent UCLM to NOAELs for insectivores, but did not remain a concern when compared to LOAELs (Table 16).

#### Additional Factors Relevant to Risk Characterization for Mammalian Wildlife

A number of site-specific factors are relevant to interpretation of results of chemical comparisons and overall risk characterization for mammalian wildlife. Additional factors were evaluated relevant to zinc, the chemical for which 95 percent UCLM exceeded TRVs. Evaluation of the factors identified in Section 2.7.3, include the following:

- **Site-specific bioavailability and toxicity**—Soil surveys for the area around AOC-4 (CSRL 2014) indicate that soils tend to be moderately alkaline. Zinc demonstrates lower bioavailability and toxicity in moderately alkaline soils. Uptake factors and benchmarks for mammals are derived from studies focused on moderately to highly bioavailable concentrations of metals. Therefore, bioavailability and toxicity associated with zinc is likely to be over-estimated.
- **Habitat quality**—As discussed in the CSM, the Site provides poor quality habitat for wildlife, with little vegetation and few resources to support prey items such as soil invertebrates. The shrew has an average home range of 0.7 to 4.4 acres, and with the small size of AOC-4 and lack of suitable habitat for soil invertebrates, the shrew is likely to forage outside of the Site, and AOC-4 is likely to provide habitat for a very small population of mammals.
- **Future land use**—Based on the Site setting, future land use is likely to remain industrial. Should attempts be made to restore higher quality habitat, major physical changes to the Site's substrates would be required that would greatly alter exposure concentrations.
- **Background concentrations**—The AOC-4 maximum detected concentration of zinc did not exceed the 95% UPL background concentrations, and is therefore unlikely to warrant consideration in risk management.

#### Risk Characterization for Mammalian Wildlife

When 95 percent UCLM are compared to NOAELs protective of mammalian receptors, cadmium and zinc are found in exceedance. When 95 percent UCLM are compared to LOAELs protective of mammalian receptors, no chemicals are found in exceedance. However, a number of factors identify that the potential for risk from these metals is minimal for AOC-4. In specific, metal bioavailability and toxicity is likely over-estimated; site habitats are subject to non-chemical factors that limit their use by mammals as a resource, and would require extensive alteration to support higher quality habitat; and exceedances are limited in spatial distribution. Moreover, concentrations of one of the two metals identified are consistent with background concentrations and would not warrant risk management.

#### 2.9 UNCERTAINTY EVALUATION

This ERA for AOC-4 incorporates a number of uncertainties associated with the estimates of ecological risk. As directed in the ERA guidance (EPA 1997), a conservative approach was utilized in the ERA to ensure that chemicals eliminated from consideration do not pose risks to ecological receptors. Accordingly, the risks are likely to be overestimated. The main areas of uncertainty associated with the ERA are grouped under the following categories, each of which is discussed in the following subsections:

- Environmental Sampling and Analysis
- Analysis of Chemical Data
- Analysis of Estimated Exposure and Toxicity Data
- Assessment of Risks.

#### **Environmental Sampling and Analysis**

Of the potential uncertainties associated with the environmental sampling at AOC-4, the sample design is likely to have the greatest impact on the evaluation of risks to ecological resources. The sample design was developed based on the available historical information regarding the activities that took place at the Site and the apparent health of the ecosystem at the time of sampling. Focusing the study design to provide analyses for certain chemicals to specific suspected source areas is a valid and accepted means of maintaining a practical and efficient limit on the field effort. However, there is always a possibility that the study design could miss samples where these chemicals are present, or miss other types of chemicals in a specific sample. In an effort to address the uncertainties just discussed, and in accordance with the conservative nature of SLERAs, samples were biased to areas of likely contamination in an effort to characterize the areas that were most impacted from historic activities. For example, the food webs assume that the America robin and shrew obtain all their food from within AOC-4, clearly a highly conservative assumption. With the exception of fixed or limited mobility receptors (e.g., benthic organisms), ecological receptors are unlikely to utilize only those areas of highest contamination, and are more likely to forage over a larger area that includes areas of contamination as well as less contaminated outlying areas.

### **Analysis of Chemical Data**

The maximum concentration of a pair of duplicate or split samples (taken from the same location on the same date) was used to represent the concentration for that location. Selecting the maximum concentration of a chemical detected in duplicate samples for use in the ERAs is a conservative measure and may overestimate risks. The 95 percent UCLM was used as an upper estimate of mean exposures. This exposure scenario is conservative and may also overestimate risks presented in this report.

Chemicals that are not detected in any onsite samples are considered not to be present at the Site, because, based on the analytical tools and capabilities at the time of investigation, there is no evidence indicating that these chemicals are present. Risks from these non-detected chemicals cannot be determined; therefore, the assessment of risk from these non-detected chemicals remains an uncertainty in this ERA.

#### **Analysis of Estimated Exposure and Toxicity Data**

A major source of uncertainty in the SLERA is associated with the estimation of receptor exposure to COPECs. Generally, the models used to estimate exposures from soil and prey were created to represent a worst-case scenario of possible risks to the receptor groups, and thus, many conservative assumptions were incorporated into the models. For example, bioaccumulation of a chemical in a prey organism was estimated from the maximum detected concentration in soil. Also, a BAF of 1.0 was used to estimate chemical concentrations in prey (soil invertebrates) for which literature-based BAFs were not available. This accumulation factor is expected to provide a conservative estimate of accumulation for all chemicals that are not bioaccumulative. Additionally, for the SLERA, the models assume that receptors are exposed to the maximum detected concentration of chemicals over their entire foraging range. This approach is consistent with the objectives of the screening-level assessment, which is to estimate a worst-case scenario under which risks would not be underestimated. It is expected, however, that such a conservative scenario would overestimate risk.

There is uncertainty associated with the lack of formal literature-based TRVs for certain chemicals. There were a number of semivolatile and volatile chemicals detected (Table 5) for which TRVs could not be established or derived for some chemicals because adequate toxicity information could not be found in the scientific literature. Given the absence of methods for estimating risks from exposure to chemicals with no appropriate TRVs, it is not possible to estimate the uncertainty associated with the limitation. It is not possible to indicate if the impacts result in an underestimate or overestimate of potential ecological risks. Presumably, either scenario is possible. Consequently, risks to ecological receptors resulting from exposure to these chemicals without TRVs cannot be quantitatively assessed.

There is also uncertainty associated with toxicological evaluation of essential nutrients including calcium, iron, magnesium, potassium, and sodium. These chemicals are necessary for metabolic

processes in organisms and, thus, are considered essential nutrients for wildlife. At naturally occurring concentrations, receptors are able to regulate uptake and metabolism of these elements. However, as with all chemicals, it is possible that nutrients may produce toxic effects at very highly elevated concentrations. These five chemicals do not have screening level concentrations or TRVs, except iron which has screening level concentrations for surface soil. As these metals are essential nutrients, adverse effects on organisms can occur if concentrations are either too low (causing deficiency symptoms) or too high (causing toxic symptoms). However, organisms can adapt to different levels of these metals, although there is little information available regarding concentrations at which adverse effects of either type may be observed. Because screening-level concentrations and TRVs are not available for the essential nutrients, it is not possible to quantitatively assess the potential for risks to ecological receptors from them. However, because these nutrients are essential to flora and fauna, these essential nutrients are not maintained as COPECs.

#### **Assessment of Risks**

There are uncertainties associated with the assessment of risks in the ERA for the Site. One apparent uncertainty results from the extrapolation of assumptions about the potential for adverse effects from individual organisms to populations. The intent of this ERA, as set forth in the assessment endpoints, is to ultimately evaluate risks to populations. Few methods are available to extrapolate the potential for adverse effects from the individual level to the population level. It is generally assumed that if there is no potential for direct adverse effects to individual organisms then it is also unlikely for there to be the potential for direct adverse effects to populations. Similarly, it is assumed that if there is the potential for adverse effects to individual organisms there is also the potential for adverse effects to populations. However, it is conservative to assume that potential damage at the individual level will impact the populations in the surrounding ecosystem.

This uncertainty is one of several limitations associated with the use of HQs to determine the potential for risk to ecological receptors. While the HQ is a standard tool in ERAs set forth in EPA guidance (EPA 1997), an article in the scientific literature points out a number of limitations to the use of this method (Tannenbaum et al. 2003). The use of the HQ identifies a potential for risk as opposed to an actual risk, because the HQ result is not a probability. Because the HQ identifies whether a dose or concentrations exceeds a benchmark, it is not a linear or scalable metric. Also, the HQ cannot be used to quantitatively extrapolate between individual and population level effects. Because HQs are based on NOAELs and on the most sensitive species in a media, HQs are often exceeded by concentrations normally found in the environment. All of these limitations should be considered before using HQ-based estimates of the potential for risk to draw conclusions or make decisions based on assessment results.

Another important uncertainty is the limited ability of risk assessment to assess combined and synergistic effects of chemicals. At the Site, ecological receptors are exposed to a chemical mixture; however, comparison of individual chemicals to TRVs does not capture the potential for combined effects. Combined and synergistic effects are usually assessed by performing

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bioassays. As such, risk assessment conclusions have conservatively identified the potential for synergistic effects, and recommended in certain cases the consideration in risk management of all detected chemicals.

In addition, the assessment of risks was primarily based on the comparison of estimated doses to toxicity values from the literature. There are many uncertainties associated with these evaluation tools and thus, with the assessment of risks based upon them.

#### 3. CONCLUSIONS

A conceptual model was developed for the Site based on review of site conditions and available data. This model identified that the Site may provide limited terrestrial habitats. Based on the conceptual model, assessment endpoints were selected to represent the most sensitive of ecological receptors within AOC-4's ecological community. The assessment endpoints included the survival, growth, and reproduction of plants, soil invertebrates, insectivorous birds, and insectivorous mammals.

Assessment endpoints were defined to reflect the potential impacts of complete and significant exposure pathways discussed above and to aid in identifying representative receptor species. These endpoints included the viability of the soil invertebrate community as resources for wildlife. Measurement endpoints were selected to provide a quantifiable means of characterizing risks. The measurement endpoints for plant and soil invertebrates included an initial comparison of maximum concentrations to media-specific screening criteria to identify potential COPECs. Maximum and 95 percent UCLM EPCs were then compared to receptor specific benchmarks. The benchmarks selected are highly precautionary and thus provide a conservative assessment of site risks. Due to the small size and nature of the disturbed habitat at AOC-4, comparison of the 95 percent UCLM concentrations to TRVs and LOAELs was given the strongest weight of evidence.

Maximum concentrations were initially compared to media-specific screening criteria to identify potential COPECs. For higher trophic level wildlife, additional measurement endpoints were based on the results of food web models that predict the dose of chemicals ingested by wildlife. These doses were then compared to benchmarks. The first measurement endpoint evaluated was a screening level comparison of maximum case scenario doses to no-effects benchmarks. Additional measurement endpoints included comparison of 95 percent UCLM case scenario doses to NOAELs and LOAELs.

To test the measurement endpoints, both site-specific and literature-based information were used to develop exposure and toxicity data and assumptions for use in estimating risks. These tools were used in the data evaluation to test each measurement endpoint as a line of evidence. Additional considerations specific to AOC-4 were also taken into consideration, such as the size of the Site, the current use, and the home range of wildlife receptors. Lines of evidence were combined in a qualitative weight-of-evidence discussion to determine the potential for risks. Several metals had 95 percent UCLM concentrations higher than TRVs and LOAEL HQs greater or equal to 1.0 for the receptors. Exceedances include:

- **Terrestrial plants**—When 95 percent UCLM are compared to TRVs protective of terrestrial plants, barium, chromium, mercury, vanadium, and zinc are found in exceedance.
- **Soil invertebrates**—When 95 percent UCLM are compared to TRVs protective of soil invertebrates, barium, chromium, mercury, and zinc are found in exceedance.

- **Avian wildlife**—When 95 percent UCLM are compared to NOAELs protective of avian receptors, barium, cadmium, copper, lead, vanadium, and zinc are found in exceedance. When 95 percent UCLM are compared to LOAELs protective of avian receptors, vanadium and zinc are found in exceedance.
- Mammalian wildlife—When 95 percent UCLM are compared to NOAELs protective of mammalian receptors, zinc is found in exceedance. When 95 percent UCLM are compared to LOAELs protective of mammalian receptors, no chemicals are found in exceedance.

However, a number of factors identify that the potential for risk from these metals is minimal for AOC-4. Specifically, metal bioavailability and toxicity is likely over-estimated; site habitats are subject to non-chemical factors that limit habitat quality and would require extensive alteration to support higher quality habitat; and exceedances are limited in spatial distribution.

The maximum detected concentrations of barium, chromium, lead, and zinc did not exceed the 95% UPL background concentrations and would not warrant risk management. The vanadium 95 UCL (17 mg/kg) does not exceed the 95 UPL background, nor the Texas-specific soil background concentration (50 mg/kg; TCEQ 2014b) value; consequently, vanadium does not warrant risk management. The copper NOAEL HQ is just over one (HQ NOAEL 1.01) and the LOAEL HQ is well below one (0.07), so risks are acceptable.

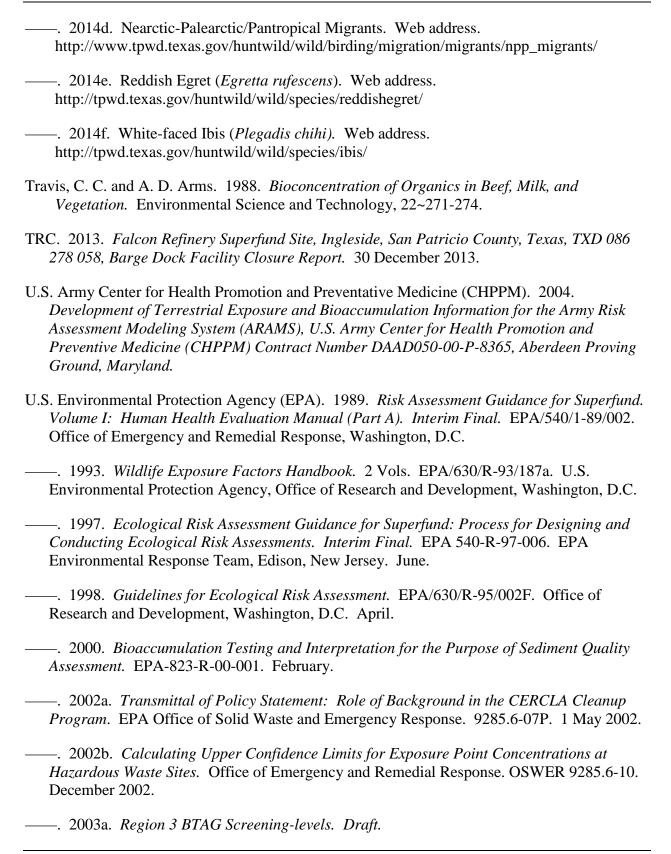
The only remaining COPEC is mercury with HQs for terrestrial plants and soil invertebrates at 3.9 and 12, respectively. The maximum detected concentration was 1.5 mg/kg in sample SO4-01, which is three times the next highest concentration (0.47 mg/kg). Both site-specific and Texas-specific background values (0.02-0.04 mg/kg) are lower than any measured mercury at the site. While mercury concentrations at AOC 4 are high compared to background, they are not particularly high considering that the site is a disturbed industrial property. Site use is expected to preclude the area from being used as viable ecological habitat for plants and soil invertebrates, and use of the area is not expected to change in the future. Consequently, risk management of the site for mercury is not necessary at this time. Should site use be changed and the area becomes a viable habitat, then additional assessment for potential mercury risks should be considered.

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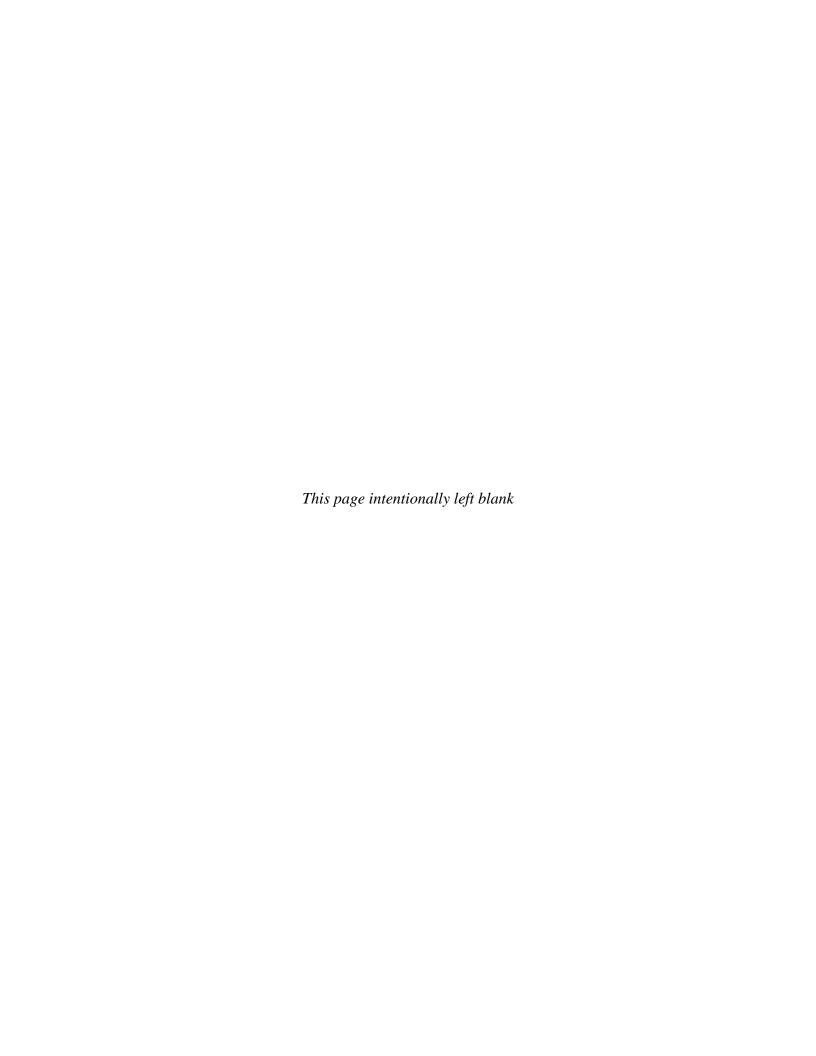
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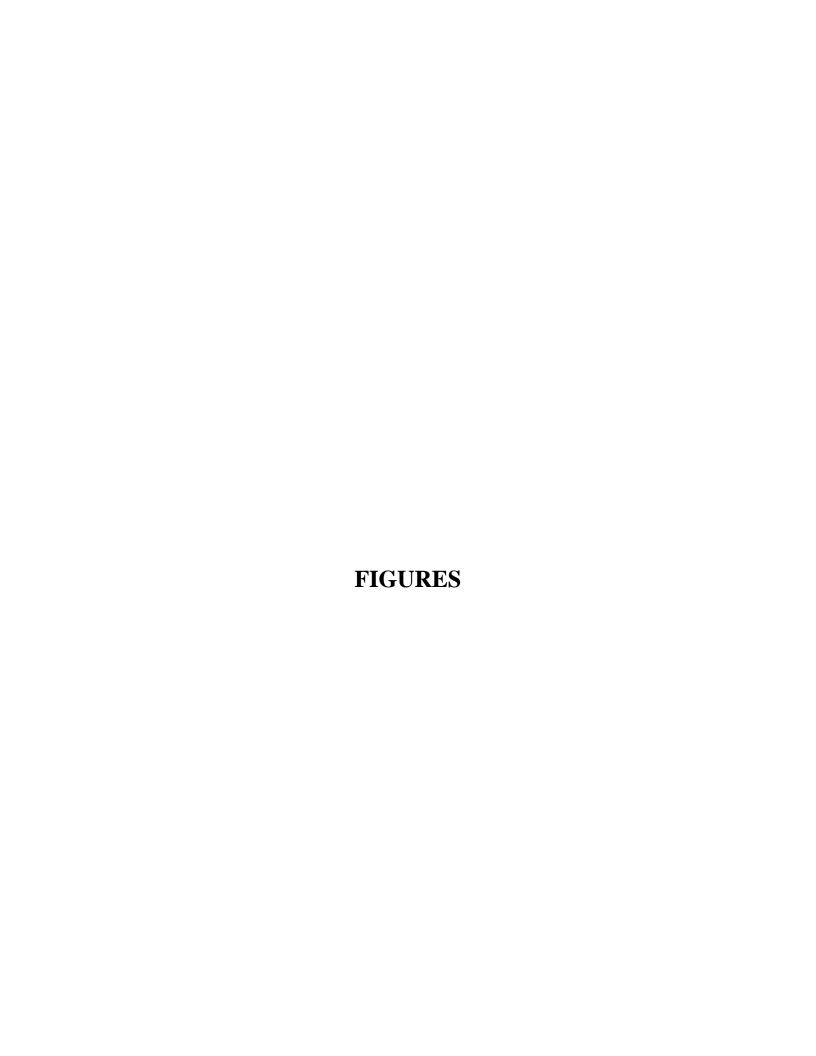




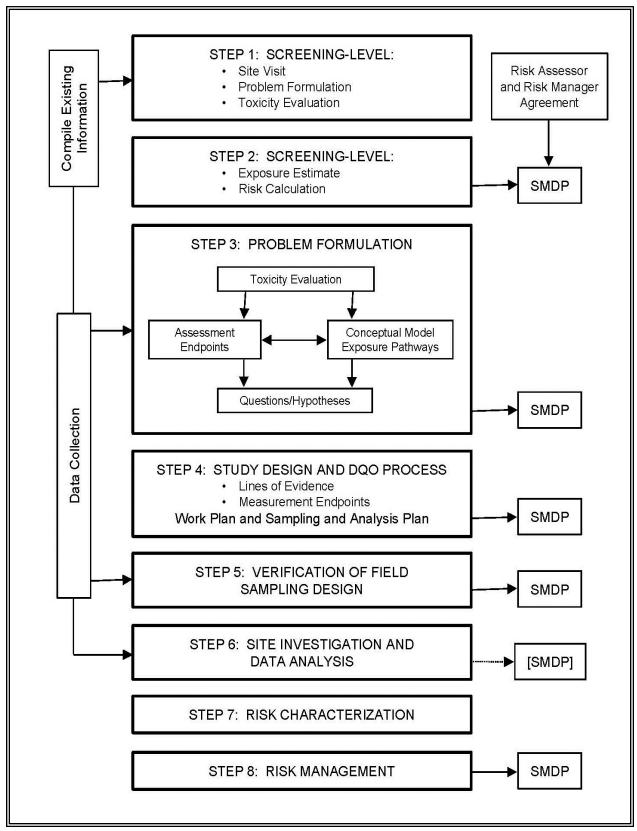


Figure 1 Location Map Ecological Risk Assessment for AOC-4









SMDP = Scientific Management Decision Points

Figure 3. Eight-step Ecological Risk Assessment Process for Superfund (from EPA 1997).





Falcon Refinery Superfund Site Ingleside, San Patricio County, Texas

Figure 4
AOC-4 Sample Locations
Ecological Risk Assessment for AOC-4

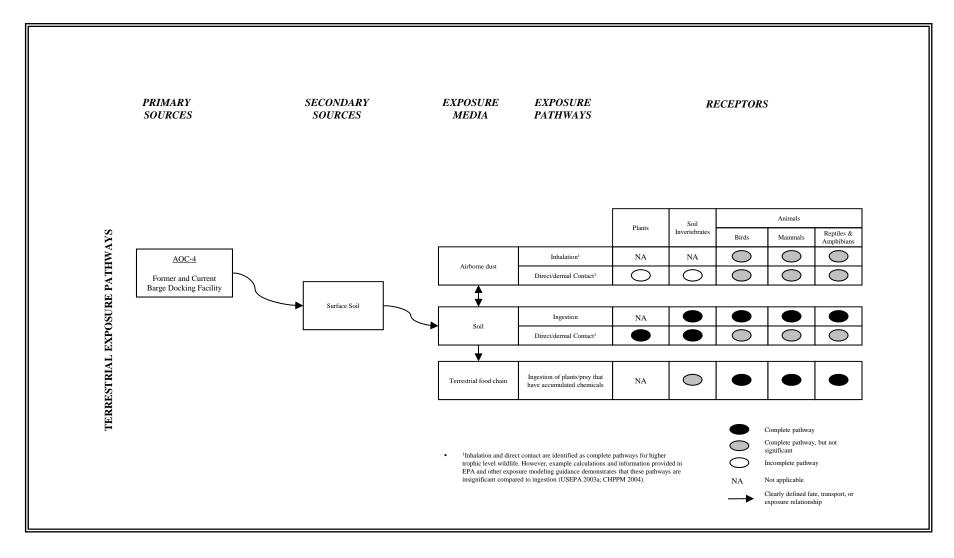
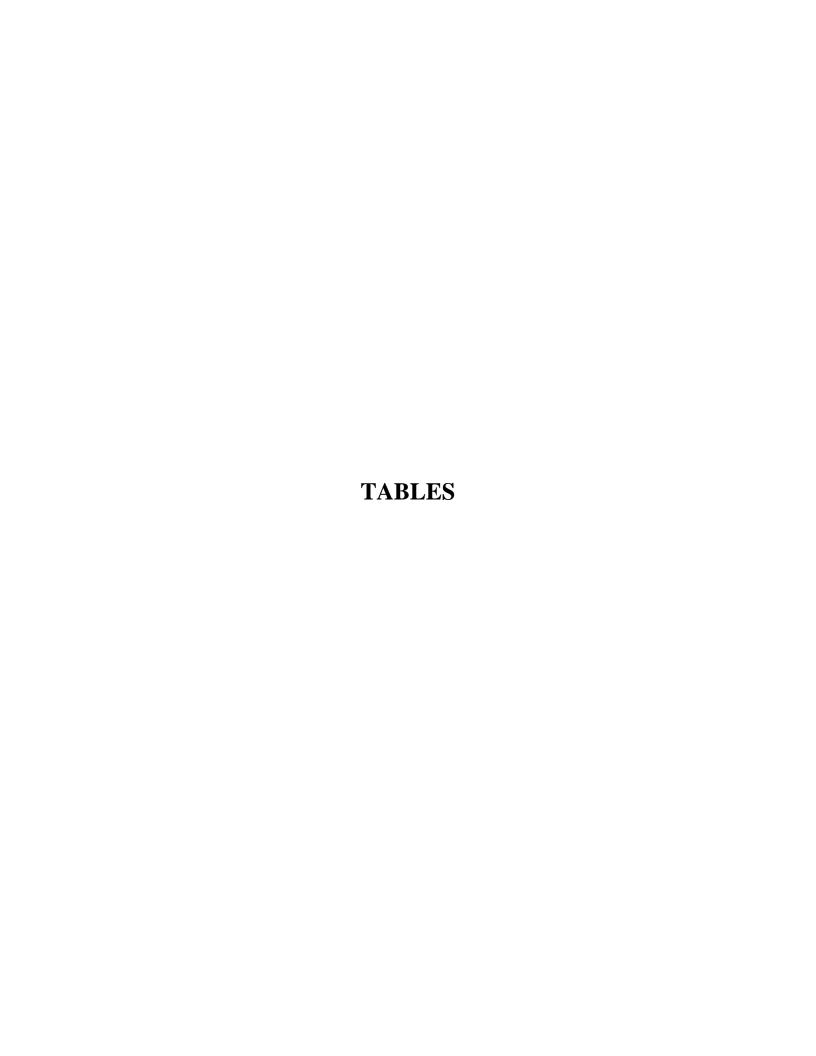
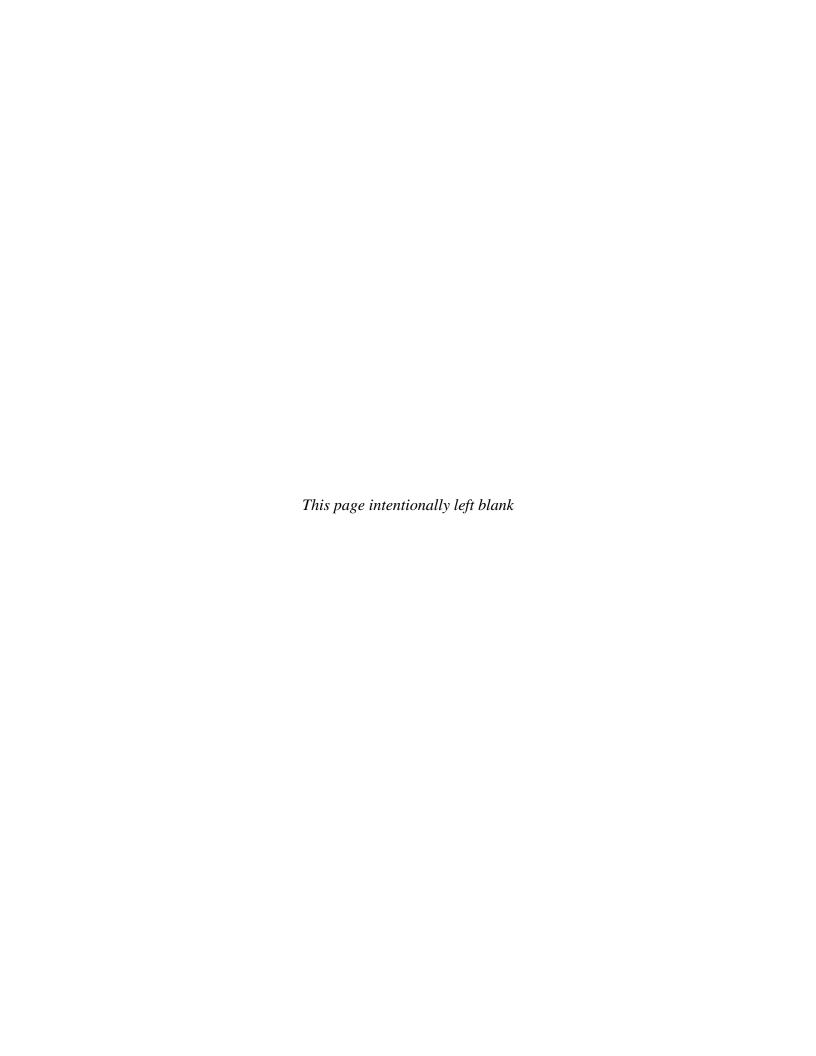


Figure 5. Ecological Conceptual Site Model for Falcon Refinery Superfund Site





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Table 1
Samples Used in the Ecological Risk Assessment

Area	Media	Sample Date	Sample ID		
		10-Sep-13	MW-17-0.0-0.5		
		10-Sep-13	SO4-01-0.0-0.5		
AOC 4	Surface	10-Sep-13	SO4-02-0.0-0.5		
AOC-4	Soil	10-Sep-13	SO4-03-0.0-0.5		
		10-Sep-13	SO4-04-0.0-0.5		
		10-Sep-13	SO4-05-0.0-0.5		
NOTE:					
AOC = Area of Concern					

Table 2
Measurement Endpoints for Ecological Risk Assessment

Assessment Endpoint	Measurement Endpoint	On Site-Measurements/Exposure Point Concentrations (EPC)	Evaluation Method	Risk Indicators
Assessment Endpoint		( - 7		
Protection of terrestrial plants	Initial screening	Surface soil concentrations measured at site during recent sampling	Direct companson to the Eco-SSL or Region IV ecological screening values to define COPECs	Chemicals defined as COPECs indicate the potential for risk
and surface soil invertebrates exposed to COPECs in surface soil from adverse survival, growth and reproductive effects	Comparison of surface soil concentrations to benchmarks	Surface soil concentrations measured at site during recent sampling     SLERA: Maximum Concentrations     Refined BRAPF: Mean Concentrations	Direct comparison of maximum surface soil concentrations to plant benchmarks (TRVs) Direct comparison of maximum surface soil concentrations to invertebrate benchmarks (TRVs) Direct comparison of mean surface soil concentrations and individual concentrations to invertebrate benchmarks Invertebrate benchmarks from EPA Eco-SSLs; ORNL benchmarks (Efroymson et al., 1997b)	Exceedence of benchmarks indicates potential for risks
	Initial screening	Surface soil concentrations measured at site during recent sampling	Direct comparison to the Eco-SSL or Region IV ecological screening values to define COPECs	Chemicals defined as COEPCs indicate the potential for risk
Protection of terrestrial mammals and birds to ensure that ingestion of COPCs in surface soil and food do not have unacceptable impacts on survival, growth, and reproduction	Comparison of modeled food web doses to benchmarks	Surface soil concentrations measured at site during recent sampling  LERA: Maximum Concentrations Refined SLERA & BRAPF: Mean Concentrations Ingested dose based on literature-based exposure factors and uptake equations  SLERA: Maximum Dose Refined SLERA & BRAPF: Mean Dose	Calculate maximum case scenario doses using food web models and compare to no-effects benchmarks Calculate mean case scenario doses and compare to no-and low-effects benchmarks Mammal and bird dose-based benchmarks from  USEPA EcoSSL ORNL benchmarks (Sample et al., 1998b)  Additional literature-based sources as relevant	Exceedence of benchmarks indicates a potential for risks
	Qualitative evaluation of habitat	Species lists and observations from previous habitat surveys     Observations of vegetation community distribution from aerial photographs	Presence of signs of stress, such as bare areas	Presence of signs of stress indicates potential impacts/risks
Protection of reptiles and amphibians to ensure that ingestion of COEPCs in surface soil and food do not have unacceptable impacts on survival, growth, and reproduction	Comparison of modeled food web doses to benchmarks	EPCs evaluated for other receptors	Evaluate whether other wildlife receptors are at risk and consider results as surrogate for reptiles and amphibians.	Risks from COPECs to other receptors indicate that there may be a risk to reptiles and amphibians from the same COEPCs
NOTE: BRAPF = Baseline Risk Assessm	ent Problem Formulation	•	•	

COPEC = Chemical of Potential Ecological Concern

Eco-SSL = Ecological Soil Screening Levels

NAWQC = National Ambient Water Quality Criteria

 $ORNL = Oak\ Ridge\ National\ Laboratory$ 

SLERA = Screening Level Ecological Risk Assessment

TRV = Toxicity Reference Value

EPA = U.S. Environmental Protection Agency

Table 3
Ecological Screening Benchmarks

Ecological Screening Dencimarks					
Chemical	Soil Criteria (mg/kg)	Soil Criteria Source			
Metals					
Aluminum	5.00E+01	Region 4, Retain only if soil pH < 5.5 (TCEQ)			
Antimony	2.70E-01	Mammalian Eco-SSL			
Arsenic	1.80E+01	Plant Eco-SSL			
Barium Beryllium	3.30E+02 1.00E+01	Soil Invertebrate Eco-SSL  TCEQ Plant Eco-SSL			
Cadmium	3.60E-01	Mammalian Eco-SSL			
Calcium	NA				
Chromium	4.00E-01	TCEQ Plant Eco-SSL			
Cobalt	1.30E+01	Plant Eco-SSL			
Copper	2.80E+01	Avian Eco-SSL			
Iron Lead	2.00E+02	Region 4 Avian Eco-SSL			
Magnesium	1.10E+01 NA	Aviaii Eco-SSL			
Manganese	2.20E+02	Plant Eco-SSL			
Mercury	1.00E-01	TCEQ Soil Invertebrate Eco-SSL			
Nickel	3.80E+01	Plant Eco-SSL			
Potassium	NA				
Selenium	5.20E-01	Plant Eco-SSL			
Silver Sodium	4.20E+00 NA	Avian Eco-SSL			
Thallium	1.00E+00	TCEQ Plant Eco-SSL			
Vanadium	2.00E+00	TCEQ Plant Eco-SSL			
Zinc	4.60E+01	Avian Eco-SSL			
Polynuclear Aromatic Hydrocar	bons				
2-Methylnaphthalene	NA				
Acenaphthene	2.00E+01	TCEQ Plant Eco-SSL			
Acenaphthylene	NA				
Anthracene	NA				
Benzo(a)Anthracene	NA				
Benzo(a)Pyrene	NA				
Benzo(b)Fluoranthene	NA				
Benzo(g,h,i)Perylene	NA				
Benzo(k)Fluoranthene	NA				
Chrysene	NA				
Dibenzo(a,h)Anthracene	NA				
Fluoranthene	NA				
Fluorene	3.00E+01	TCEQ Soil Invertebrate Eco-SSL			
Indeno(1,2,3-Cd)Pyrene	NA				
Naphthalene	NA NA				
Phenanthrene	NA NA				
	+				
Pyrene Total I MW DAHs	NA 2 90F   01	 Soil Invertebrate Eco SSI			
Total LMW PAHs Total HMW PAHs	2.90E+01 1.10E+00	Soil Invertebrate Eco-SSL Mammalian Eco-SSL			
Semivolatile Organic Compound		Manimum Leo DDL			
	6.00E+01	TCEQ Plant Eco-SSL			
2-Methylphenol	NA				
4-Methylphenol	NA NA				
Acetophenone	NA NA				
	+				
Benzaldehyde	NA NA				
Benzoic Acid	NA NA	<del></del>			
Butyl benzyl phthalate	NA				
Bis(2-ethylhexyl)phthalate	NA				
Caprolactum	NA				
Carbazole	NA				

Table 3
Ecological Screening Benchmarks

Chemical	Soil Criteria (mg/kg)	Soil Criteria Source	
Diethyl phthalate	1.00E+02	TCEQ Plant Eco-SSL	
	2.00E+02	TCEQ Frant Eco-SSL  TCEQ Soil Invertebrate Eco-SSL	
Dimethyl phthalate			
Di-N-Butyl phthalate	2.00E+02	TCEQ Plant Eco-SSL	
Di-N-octyl Phthalate	NA		
Isophorone	NA		
Phenol	5.00E-02	Region 4	
Volatile Organic Compounds			
1,1,2,2-Tetrachloroethane	NA		
1,2,4-Trimethlybenzene	NA		
1,3,5-Trimethylbenzene	NA		
2-Butanone	NA		
4-Methyl-2-pentanone	NA		
Acetone	NA		
Benzene	5.00E-02	Region 4	
Benzaldehyde	1.00E-02	Region 4	
Carbon disulfide	NA		
Chloroform	1.00E-03	Region 4	
Chloromethane	NA		
Ethylbenzene	5.00E-02	Region 4	
Isopropylbenzene	NA		
Methylene chloride	NA		
n-Propylbenzene	NA		
Styrene	1.00E-01	Region 4	
Tetrachloroethene	1.00E-02	Region 4	
Toluene	5.00E-02	Region 4	
Trichloroethene	NA		
Trichloroflouromethane	NA		
Xylenes (m & p)	NA		
Xylenes (o)	NA		
Xylenes (Total)	5.00E-02	Region 4	

Sources: The lowest Eco-SSL available from one of the following:

- $(1) Texas\ Commission\ on\ Environmental\ Quality\ (TCEQ)\ -\ Table\ 3.4,\ accessed\ at\ http://www.tceq.texas.gov/assets/public/remediation/trrp/rg263-draft.pdf$
- (2) EPA Eco-SSLs, accessed at http://www.epa.gov/ecotox/ecossl
- (3) EPA Region 4 Ecological Screening Values, accessed at http://www.epa.gov/region4/superfund/programs/riskassess/ecolbul.html

#### NOTE:

Eco-SSL = Ecological Soil Screening Levels

EPA = U.S. Environmental Protection Agency

 $HMW\ PAH = High\ molecular\ weight\ polynuclear\ aromatic\ hydrocarbon$ 

 $LMW\ PAH = Low\ molecular\ weight\ polynuclear\ aromatic\ hydrocarbon$ 

 $mg/kg = Milligram \; per \; kilogram$ 

NA = Screening value not available

# Table 4 Maximum Soil Detection Comparison to Screening Levels for AOC-4

					Selection of Chemical
		ç	rface Soil		of Potential Ecological Concern
		Sul	riace Soil	Screening	Concern
	Frequency	Maximum	Location of	Criteria	
Analyta	of Detection	(mg/kg)	Maximum	(mg/kg)*	Terrestrial Habitats
Analyte  Metals	or Dettetton	(111g/11g)		(111g/11g)	201100011111111110111110
Aluminum	6/6	1.70E+04	SO4-01-0.0-0.5	pH < 5.5	NO
Arsenic	6//6	5.70E+00	SO4-01-0.0-0.5	1.80E+01	NO
Barium	6/6	8.09E+02	SO4-01-0.0-0.5	3.30E+02	YES
Cadmium	1/6	9.00E-01	SO4-01-0.0-0.5	3.60E-01	YES
Calcium	6/6	2.64E+05	SO4-03-0.0-0.5	NA	NO, Esn. Nut.
Chromium	6/6	1.76E+01	SO4-04-0.0-0.5	4.00E-01	YES
Cobalt	6/6	3.80E+00	SO4-01-0.0-0.5	1.30E+01	NO
Copper	6/6	3.98E+01	SO4-04-0.0-0.5	2.80E+01	YES
Iron	6/6	1.30E+04	SO4-01-0.0-0.5	pH < 5.5	NO
Lead	6/6	<b>4.30E+01</b> 6.01E+03	SO4-01-0.0-0.5 SO4-01-0.0-0.5	1.10E+01 NA	YES
Magnesium Manganese	6/6 <b>6/6</b>	2.59E+02	SO4-01-0.0-0.5	2.20E+02	NO, Esn. Nut. YES
Mercury	6/6	1.50E+00	SO4-01-0.0-0.5	1.00E-01	YES
Nickel	6/6	1.85E+01	SO4-01-0.0-0.5	3.80E+01	NO
Potassium	6/6	4.00E+03	SO4-01-0.0-0.5	NA	NO, Esn. Nut.
Sodium	5/6	4.23E+03	MW-17-0.0-0.5	NA	NO, Esn. Nut.
Vanadium	6/6	2.13E+01	SO4-01-0.0-0.5	2.00E+00	YES
Zinc	6/6	5.60E+02	SO4-01-0.0-0.5	4.60E+01	YES
Polynuclear Aromatic Hydrocarbons					
Acenaphthene	3/6	3.20E-02	SO4-04-0.0-0.5	2.00E+01	NO
Acenaphthylene	4/6	6.10E-02	SO4-04-0.0-0.5	NA	Use Total LMW
Anthracene	5/6	6.50E-02	SO4-04-0.0-0.5	NA NA	Use Total LMW
Benzo(a)Anthracene Benzo(a)Pyrene	6/6 6/6	5.90E-01 5.09E-01	MW-17-0.0-0.5 MW-17-0.0-0.5	NA NA	Use Total HMW Use Total HMW
Benzo(a)Fyrene Benzo(b)Fluoranthene	6/6	8.20E-01	MW-17-0.0-0.5	NA NA	Use Total HMW
			SO4-04-0.0-0.5		
Benzo(g,h,i)Perylene	6/6	2.19E-01	MW-17-0.0-0.5	NA	Use Total HMW
Benzo(k)Fluoranthene	6/6	2.70E-01	SO4-04-0.0-0.5	NA	Use Total HMW
Chrysene	6/6	6.00E-01	MW-17-0.0-0.5	NA	Use Total HMW
Dibenzo(a,h)Anthracene	5/6	7.60E-02	MW-17-0.0-0.5	NA	Use Total HMW
Fluoranthene	6/6	1.40E+00	MW-17-0.0-0.5	NA	Use Total LMW
Fluorene	2/6	1.50E-02	MW-17-0.0-0.5	3.00E+01	NO
Indeno(1,2,3-Cd)Pyrene	6/6	3.50E-01	SO4-04-0.0-0.5	37.	Use Total HMW
	616	2.500.01	MW-17-0.0-0.5	NA NA	II T. (-1 I MW
Phenanthrene Pyrene	6/6 6/6	3.50E-01 1.10E+00	MW-17-0.0-0.5 MW-17-0.0-0.5	NA NA	Use Total LMW Use Total HMW
Total LMW PAHs	6/6	4.49E-01	MW-17-0.0-0.5	2.90E+01	NO NO
Total HMW PAHs	6/6	5.87E+00	MW-17-0.0-0.5	1.10E+00	YES
Semivolatile Organic Compounds					
Acetophenone	1/6	6.20E-02	SO4-05-0.0-0.5	NA	YES
Benzaldehyde	1/6	6.60E-02	SO4-05-0.0-0.5	NA	YES
Bis(2-ethylhexyl)phthalate	2/6	2.20E-01	SO4-04-0.0-0.5	NA NA	YES
			SO4-05-0.0-0.5	1	
Carbazole	1/6	1.90E-02		NA	YES
Dimethyl phthalate	2/6	1.50E-01	SO4-04-0.0-0.5	2.00E+02	NO
Phenol	1/6	3.30E-02	SO4-05-0.0-0.5	5.00E-02	NO
Volatile Organic Compounds					
2-Butanone	1/6	1.40E-02	SO4-01-0.0-0.5	NA	YES
Ethylbenzene	1/6	3.70E-03	SO4-01-0.0-0.5	5.00E-02	NO
Isopropylbenzene	1/6	3.30E-04	SO4-01-0.0-0.5	NA	YES
Tetrachloroethene	1/6	1.20E-03	SO4-01-0.0-0.5	1.00E-02	NO
Trichloroflouromethane	4/6	5.00E-04	SO4-01-0.0-0.5	NA	YES
Xylenes (m & p)	2/6	3.50E-02	SO4-01-0.0-0.5	1	
			SO4-01-0.0-0.5	NA NA	YES YES
Xylenes (o)	1/6	1.20E-02	504 01-0.0-0.5	NA	1 E3

NOTE:

\* See Table 3

Esn. Nut. = Essential nutrient

 $HMW\ PAH = High\ molecular\ weight\ polynuclear\ aromatic\ hydrocarbon$   $LMW\ PAH = Low\ molecular\ weight\ polynuclear\ aromatic\ hydrocarbon$ 

mg/kg = Miligram per kilogramNA = Screening value not available

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Table 5
Frequency of Detection and Exposure Point Concentrations for AOC-4

Surface Soil				
	Maximum	95% UCL Mean		
Frequency	(mg/kg)	(mg/kg)		
6/6	8.09E+02	5.32E+02		
1/6	9.00E-01	9.00E-01		
	1.76E+01	1.76E+01		
6/6	3.98E+01	3.98E+01		
6/6	4.30E+01	3.98E+01		
		1.85E+02		
		1.18E+00		
		1.83E+01		
6/6	5.60E+02	4.33E+02		
rbons				
6/6	5.87E+00	4.34E+00		
ıds				
1/6	6.20E-02	6.20E-02		
1/6	6.60E-02	6.60E-02		
2/6	2.20E-01	2.20E-01		
1/6	1.90E-02	1.90E-02		
Volatile Organic Compounds				
1/6	1.40E-02	1.40E-02		
1/6	3.30E-04	3.30E-04		
4/6	5.00E-04	4.40E-04		
2/6	3.50E-02	3.50E-02		
1/6	1.20E-02	1.20E-02		
	1/6 6/6 6/6 6/6 6/6 6/6 6/6 6/6 6/6 6/6	Maximum (mg/kg)		

NOTE:

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

LMW PAH = Low molecular weight polynuclear aromatic hydrocarbon

mg/kg = Milligram per kilogram

UCL = Upper confidence level

Table 6 Uptake Models Relating Concentrations in Soil to Concentrations in Soil Invertebrates

	Food Item (Worm) Uptake				
Chemical	Uptake Model <sup>A, B, C</sup>	BAF/Equation (mg/kg dry wt. to mg/kg dry wt.)	Source		
Metals	optane moder	(mg/ng dry wa to mg/ng dry wa)	Source		
Aluminum	Uptake Factor	1.18E-01	90% UF, Sample et al 1998a		
Antimony	Uptake Factor	1.00E+00	Default		
-		ln(dry worm conc, mg/kg) =			
Arsenic	Log Linear	(-1.421+0.706*ln(soil conc))	Sample et al. 1998a		
Barium	Uptake Factor	1.60E-01	90% UF, Sample et al 1998a		
Beryllium	Uptake Factor	1.18E+00	90% UF, Sample et al 1998a		
Cadmium	Log Linear	ln(dry worm conc, mg/kg) =	Sample et al. 1998a		
	_	(2.114+0.795*ln(soil conc))			
Calcium	Uptake Factor	1.00E+00	Default		
Chromium	Log Linear	ln(dry worm conc, mg/kg) = (2.481+-0.067*ln(soil conc))	Sample et al. 1998a		
Cobalt	Uptake Factor	2.91E-01	90% UF, Sample et al 1998a		
	1,	ln(dry worm conc, mg/kg) =			
Copper	Log Linear	(1.675+0.264*ln(soil conc))	Sample et al. 1998a		
Iron	Uptake Factor	7.80E-02	90% UF, Sample et al 1998a		
Lead	Log Linear	ln(dry worm conc, mg/kg) =	Sample et al. 1998a		
		(-0.218+0.807*ln(soil conc))	<u> </u>		
Magnesium	Uptake Factor	5.30E-01	90% UF, Sample et al 1998a		
Manganese	Log Linear	ln(dry worm conc, mg/kg) =	Default		
	+	(-0.809+0.682*ln(soil conc)) ln(dry worm conc, mg/kg) =			
Mercury	Log Linear	(-0.684+0.118*ln(soil conc))	Sample et al. 1998a		
		ln(dry worm conc, mg/kg) =			
Nickel	Log Linear	(3.677-0.26*ln(soil conc))	Sample et al. 1998a		
Potassium	Uptake Factor	1.00E+00	Default		
Selenium	Log Linear	ln(dry worm conc, mg/kg) =	Sample et al. 1998a		
		(-0.075+0.733*ln(soil conc))			
Silver	Uptake Factor	1.53E+01	90% UF, Sample et al 1998a		
Sodium	Uptake Factor	1.00E+00	Default		
Thallium	Uptake Factor	1.00E+00	Default		
Vanadium	Uptake Factor	8.80E-01 ln(dry worm conc, mg/kg) =	90% UF, Sample et al 1998a		
Zinc	Log Linear	(4.449+0.328*ln(soil conc))	Sample et al. 1998a		
PAHs		(4.445 + 0.526 m(50ff cone))			
2-Methylnaphthalene	Uptake Factor	2.00E-01	Beyer and Stafford 1993		
Acenaphthene	Uptake Factor	3.00E-01	Beyer and Stafford 1993		
Acenaphthylene	Uptake Factor	2.20E-01	Beyer and Stafford 1993		
Anthracene	Uptake Factor	3.20E-01	Beyer and Stafford 1993		
Benzo(a)Anthracene	Uptake Factor	2.70E-01	Beyer and Stafford 1993		
Benzo(a)Pyrene	Uptake Factor	3.40E-01	Beyer and Stafford 1993		
Benzo(b)Fluoranthene	Uptake Factor	2.10E-01	Beyer and Stafford 1993		
Benzo(g,h,i)Perylene	Uptake Factor	1.50E-01	Beyer and Stafford 1993		
Benzo(k)Fluoranthene	Uptake Factor	2.10E-01	Beyer and Stafford 1993		
Chrysene Dibenzo(a,h)Anthracene	Uptake Factor Uptake Factor	4.40E-01 4.90E-01	Beyer and Stafford 1993 Beyer and Stafford 1993		
Fluoranthene	Uptake Factor Uptake Factor	4.90E-01 3.70E-01	Beyer and Stafford 1993  Beyer and Stafford 1993		
Fluorantnene	Uptake Factor	2.00E-01	Beyer and Stafford 1993		
Indeno(1,2,3-Cd)Pyrene	Uptake Factor	4.10E-01	Beyer and Stafford 1993		
Naphthalene	Uptake Factor	2.10E-01	Beyer and Stafford 1993		
Phenanthrene	Uptake Factor	2.80E-01	Beyer and Stafford 1993		
Pyrene	Uptake Factor	3.90E-01	Beyer and Stafford 1993		
Total LMW PAHs	NA				
Total HMW PAHs	NA				
SVOCs		1007.00	7.0		
Acetophenone	Uptake Factor	1.00E+00	Default		
Benzaldehyde	Uptake Factor	1.00E+00	Default		
Bis(2-ethylhexyl)phthalate	Uptake Factor Uptake Factor	1.00E+00	Default		
Carbazole	Uptake Pactor	1.00E+00	Default		
VOCs 2-Butanone	Uptake Factor	1.00E+00	Default		
Isopropylbenzene	NA	1.00£=00	Default 		
Trichlorofluoromethane	Uptake Factor	1.00E±00	Detailit		
Trichlorofluoromethane  Xylenes (m & p)	Uptake Factor Uptake Factor	1.00E+00 1.00E+00	Default Default		

A - The default uptake factor for chemicals were no information was available was assumed to be 1.

ng/kg = Milligram per kilogram

ng/kg dry wt = Milligram per kilogram of dry weight

NA = Uptake Model not available

B - Equation types:

Uptake Factor: [ConcBio] = m x [ConcSoil] Log linear: [ConcBio] = 10b\*[ConcSoil]m

<sup>-</sup> Uptake factor derived using

ln(earthworm) = B0 + B1(ln(soil concentration))

B0 = Constituent-specific intercept based on tissue type

B1 = Constituent-specific slope based on tissue type
Data for B0 and B1 are presented in Sample, et. al 1998a, Table 12, pg. 33.

Table 7
Wildlife Exposure Factors for the Ecological Risk Assessment at AOC-4

Exposure Parameter	Value	Units	Notes
AMERICAN ROBIN			
Body Weight	0.077	kg	Value from Dunning (1984)
Food Ingestion Rate	0.22	kg dry wt./kg-day	EPA 1993, converted assuming 75% prey moisture (CHPPM 2004)
Food Ingestion Rate	0.89	kg wet wt./kg-day	EPA 1993
Incidental Soil Ingestion Rate	10.50%	% of total mass of diet	Value base on woodcock, Sample and Suter, 1994
Water Ingestion Rate	0.14	L/kg-day	EPA 1993
NORTHERN SHORT-TAILED SHREW			
Body Weight	0.015	kg	Values from Sample et al. (1996)
Food Ingestion Rate	0.16	kg dry wt./kg-day	EPA 1993, converted assuming 75% prey moisture (CHPPM 2004)
Food Ingestion Rate	0.62	kg wet wt./kg-day	EPA 1993
Incidental Soil Ingestion Rate	13.00%	% of total mass of diet	Sample and Suter, 1994
Water Ingestion Rate	0.22	L/kg-day	EPA 1993

NOTE:

CHPPM = U.S. Army Center for Health Promotion and Preventative Medicine

kg = Kilogram

kg dry wt./kg-day = Kilogram of dry weight food per kilogram of body weight per day

kg wet wt./kg-day = Kilogram of wet weight food per kilogram of body weight per day

L/kg-day = Liter of water per kilogram of body weight per day

USEPA = U.S. Environmental Protection Agency

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Table 8
Soil Toxicity Reference Values for Plants and Soil Invertebrates

	Earthworm						
	Plant Toxicity		Toxicity				
	Reference Value	Toxicity Reference Value	Reference Value	Toxicity Reference Value			
Chemical	(mg/kg dry wt)	Source and Notes	(mg/kg dry wt)	Source and Notes			
Metals							
Aluminum	5.00E+01	Efroymson et al. 1997a	NA				
Antimony	5.00E+00	Efroymson et al. 1997a	7.80E+01	EPA 2005h			
Arsenic	1.80E+01	EPA 2005b	6.00E+01	Efroymson et al. 1997b			
Barium	5.00E+02	Efroymson et al. 1997a	3.30E+02	EPA 2005e			
Beryllium	1.00E+01	Efroymson et al. 1997a	4.00E+01	EPA 2005f			
Cadmium	3.20E+01	EPA 2005b	1.40E+02	EPA 2005b			
Calcium	NA		NA				
Chromium	1.00E+00	Efroymson et al. 1997a	4.00E-01	Efroymson et al. 1997b			
Cobalt	1.30E+01	EPA 2005g	NA				
Copper	7.00E+01	EPA 2007b	8.00E+01	EPA 2007b			
Iron	NA		NA				
Lead	1.20E+02	EPA 2005c	1.70E+03	EPA 2005c			
Magnesium	NA		NA				
Manganese	2.20E+02	EPA 2007c	4.50E+02	EPA 2007c			
Mercury	3.00E-01	Efroymson et al. 1997a	1.00E-01	Efroymson et al. 1997b			
Nickel	3.80E+01	EPA 2007d	2.80E+02	EPA 2007e			
Potassium	NA		NA				
Selenium	5.20E-01	EPA 2007g	4.10E+00	EPA 2007g			
Silver	5.60E+02	EPA 2006	NA				
Sodium	NA		NA				
Thallium	1.00E+00	Efroymson et al. 1997a	NA				
Vanadium	2.00E+00	Efroymson et al. 1997a	NA				
Zinc	1.60E+02	EPA 2007e	1.20E+02	EPA 2007e			
Polynuclear Aromatic Hydrocarbons							
Total LMW PAHs	2.00E+01	Efroymson et al. 1997a, value for acenaphthene	2.90E+01	EPA 2007f			
Total HMW PAHs	2.00E+01	Efroymson et al. 1997a, value for acenaphthene	1.80E+01	EPA 2007f			
Semivolatile Organic Compounds							
Acetophenone	NA		NA				
Benzaldehyde	NA		NA				
Bis(2-ethylhexyl)phthalate	1.00E+02	Efroymson et al. 1997a, value for diethyl phthalate	2.00E+02	Efroymson et al. 1997b, value for dimethyl phthalate			
Carbazole	NA		NA				
Volatile Organic Compounds							
2-Butanone	NA		NA				
Isopropylbenzene	NA		NA				
Trichloroflouromethane	NA		NA				
Xylenes (m & p)	NA		NA				
Xylenes (o)	NA		NA				

NOTE:

EPA = U.S. Environmental Protection Agency

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

 $LMW\ PAH = Low\ molecular\ weight\ polynuclear\ aromatic\ hydrocarbon$ 

mg/kg dry wt = Milligram per kilogram of dry weight

NA = Toxicity reference value not available

### Table 9 Dose-based Toxicity Reference Values for Birds

	Avian		Avian	
	NOAEL		LOAEL	
	(mg/kg-bw	Avian NOAEL Source	(mg/kg-bw	
Chemical	day)	and Notes	day)	Avian LOAEL Source and Notes
Metals				
Aluminum	1.10E+02	Sample et al. 1996	NA	
Antimony	5.10E+00	EPA 2005h	1.28E+01	Sample et al. 1996
Arsenic	2.24E+00	EPA 2005a	7.40E+00	Sample et al. 1996
Barium	2.08E+01	Sample et al. 1996	4.17E+01	Sample et al. 1996
Beryllium	NA		NA	
Cadmium	1.45E+00	EPA 2005b	2.00E+01	Sample et al. 1996
Calcium	NA		NA	
Chromium	2.66E+00	Eco-SSL (trivalent) 2008	5.00E+00	Sample et al. 1996
Cobalt	7.61E+00	EPA 2005g	2.67E+01	Derived from Data in EPA 2005g
Copper	4.05E+00	EPA 2007b	6.17E+01	Sample et al. 1996
Iron	NA		NA	
Lead	1.63E+00	EPA 2005c	1.13E+01	Sample et al. 1996
Magnesium	NA		NA	
Manganese	9.97E+02	Sample et al. 1996	NA	
Mercury	4.50E-01	Sample et al. 1996	9.00E-01	Sample et al. 1996
Nickel	7.74E+01	Sample et al. 1996	1.07E+02	Sample et al. 1996
Potassium	NA		NA	
Selenium	5.00E-01	Sample et al. 1996	1.00E+00	Sample et al. 1996
Silver	2.02E+00	EPA 2006	6.05E+01	Derived from Data in USEPA 2006
Sodium	NA		NA	
Thallium	3.50E-01	Derived	NA	
Vanadium	3.44E-01	EPA 2005d	6.88E-01	Hill 1979 (study from Eco-SSL used to derive NOAEL)
Zinc	6.61E+01	EPA 2007e	1.31E+02	Sample et al. 1996
Polynuclear Aromatic Hydroca	rbons			
Total LMW PAHs	3.37E+00	Sample et al. 1996	3.37E+01	Sample et al. 1996
Total HMW PAHs	3.37E+00	Sample et al. 1996	3.37E+01	Sample et al. 1996
Semivolatile Organic Compoun	ds			
Acetophenone	NA		NA	
Benzaldehyde	NA		NA	
Bis(2-ethylhexyl)phthalate	1.10E+00	Sample et al. 1996	NA	
Carbazole	NA		NA	
Volatile Organic Compounds				
2-Butanone	NA		NA	
Isopropylbenzene	NA		NA	
Trichloroflouromethane	NA		NA	
Xylenes (m & p)	NA		NA	
Xylenes (o)	NA		NA	

#### NOTE:

Eco-SSL = Ecological Soil Screening Levels

EPA = U.S. Environmental Protection Agency

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

LMW PAH = Low molecular weight polynuclear aromatic hydrocarbon

LOAEL = Lowest Observed Adverse Effect Level

mg/kg dry wt = Milligram per kilogram of dry weight

NA = Toxicity reference value not available

NOAEL = No Observed Adverse Effect Level

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Table 10
Dose-based Toxicity Reference Values for Mammals

	Mammalian		Mammalian	
	NOAEL		LOAEL	
	(mg/kg-bw	Mammalian NOAEL Source	(mg/kg-bw	
Chemical	day)	and Notes	day)	Mammalian LOAEL Source and Notes
Metals				
Aluminum	1.93E+00	Sample et al. 1996	1.93E+01	Sample et al. 1996
Antimony	5.90E-02	EPA 2005h	1.25E+00	Sample et al. 1996
Arsenic	1.04E+00	EPA 2005a	1.26E+00	Sample et al. 1996
Barium	5.18E+01	EPA 2005e	4.36E+02	Derived from Data in EPA 2005e
Beryllium	5.32E-01	EPA 2005f	NA	
Cadmium	7.70E-01	EPA 2005b	1.00E+01	Sample et al. 1996
Calcium	NA		NA	
Chromium	2.40E+00	Eco-SSL (trivalent) 2008	1.31E+01	Sample et al. 1996
Cobalt	7.33E+00	EPA 2005g	1.18E+02	Derived from Data in EPA 2005g
Copper	5.60E+00	EPA 2007b	1.54E+01	Sample et al. 1996
Iron	NA		NA	
Lead	4.70E+00	EPA 2005c	8.00E+01	Sample et al. 1996
Magnesium	NA		NA	
Manganese	5.15E+01	EPA 2007c	2.84E+02	Sample et al. 1996
Mercury	1.32E+01	Sample et al. 1996	NA	
Nickel	1.70E+00	EPA 2007d	8.00E+01	Sample et al. 1996
Potassium	NA		NA	
Selenium	1.43E-01	EPA 2007g	3.30E-01	Sample et al. 1996
Silver	6.02E+00	EPA 2006	1.16E+02	Derived from Data in EPA 2006
Sodium	NA		NA	
Thallium	7.40E-03	Sample et al. 1996	7.40E-02	Sample et al. 1996
Vanadium	4.16E+00	EPA 2005d	8.31E+00	Sanchez et al. 1991 (study from Eco-SSL used to derive NOAEL)
Zinc	7.54E+01	EPA 2007f	3.20E+02	Sample et al. 1996
Polynuclear Aromatic Hydrocarbons				
Total LMW PAHs	6.56E+01	EPA 2007f	4.34E+02	Derived from data in EPA 2007f
Total HMW PAHs	6.15E-01	EPA 2007f	3.07E+00	Derived from data in EPA 2007f
Semivolatile Organic Compounds				
Acetophenone	NA		NA	
Benzaldehyde	NA		NA	
Bis(2-ethylhexyl)phthalate	1.83E+01	Sample et al. 1996	1.83E+02	Sample et al. 1996
Carbazole	NA		NA	
Volatile Organic Compounds				
2-Butanone	1.77E+03	Sample et al. 1996	4.57E+03	Sample et al. 1996
Isopropylbenzene	NA		NA	
Trichloroflouromethane	NA		NA	
Xylenes (m & p)	NA		NA	
Xylenes (o)	NA		NA	

NOTE:

Eco-SSL = Ecological Soil Screening Levels

EPA = U.S. Environmental Protection Agency

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

LMW PAH = Low molecular weight polynuclear aromatic hydrocarbon

LOAEL = Lowest Observed Adverse Effect Level

mg/kg dry wt = Milligram per kilogram of dry weight

NA = Toxicity reference value not available

NOAEL = No Observed Adverse Effect Level

Table 11
Comparison of Exposure Point Concentrations (EPCs) in Soil to Plant Toxicity Reference Values for AOC-4

		Terrestrial Plants (Surface Soil)						
Chemical	Plant Toxicity Reference Value (mg/kg dry wt)	Maximum EPC (mg/kg dry wt)	Hazard Quotient for Maximum EPC	95% UCL Mean EPC (mg/kg dry wt)	Hazard Quotient for 95% UCL Mean EPC			
Metals								
Barium	5.00E+02	8.09E+02	1.62E+00	5.32E+02	1.06E+00			
Cadmium	3.20E+01	9.00E-01	2.81E-02	9.00E-01	2.81E-02			
Chromium	1.00E+00	1.76E+01	1.76E+01	1.76E+01	1.76E+01			
Copper	7.00E+01	3.98E+01	5.69E-01	3.98E+01	5.69E-01			
Lead	1.20E+02	4.30E+01	3.58E-01	3.98E+01	3.32E-01			
Manganese	2.20E+02	2.59E+02	1.18E+00	1.85E+02	8.39E-01			
Mercury	3.00E-01	1.50E+00	5.00E+00	1.18E+00	3.92E+00			
Vanadium	2.00E+00	2.13E+01	1.07E+01	1.83E+01	9.14E+00			
Zinc	1.60E+02	5.60E+02	3.50E+00	4.33E+02	2.71E+00			
Polynuclear Aromatic Hydrocarbons								
Total HMW PAHs	2.00E+01	5.87E+00	2.93E-01	4.34E+00	2.17E-01			
Semivolatile Organic Compounds								
Acetophenone	NA	6.20E-02		6.20E-02	-			
Benzaldehyde	NA	6.60E-02		6.60E-02				
Bis(2-ethylhexyl)phthalate	1.00E+02	2.20E-01	2.20E-03	2.20E-01	2.20E-03			
Carbazole	NA	1.90E-02		1.90E-02				
Volatile Organic Compounds								
2-Butanone	NA	1.40E-02		1.40E-02				
Isopropylbenzene	NA	3.30E-04		3.30E-04	-			
Trichloroflouromethane	NA	5.00E-04		4.40E-04				
Xylenes (m & p)	NA	3.50E-02		3.50E-02				
Xylenes (o)	NA	1.20E-02		1.20E-02				

EPC = Exposure point concentrations

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

mg/kg dry wt = Milligram per kilogram of dry weight

UCL = Upper confidence level

Table 12
Comparison of Exposure Point Concentrations (EPCs) in Soil to Soil Invertebrate Toxicity Reference Values for AOC-4

Chemical	Invertebrate Toxicity Reference Value (mg/kg dry wt)	Maximum Exposure Point Concentration (mg/kg dry wt)	Hazard Quotient for Maximum EPC	95% UCL Mean Exposure Point Concentration (mg/kg dry wt)	Hazard Quotient for 95% UCL Mean EPC
Metals					
Barium	3.30E+02	8.09E+02	2.45E+00	5.32E+02	1.61E+00
Cadmium	1.40E+02	9.00E-01	6.43E-03	9.00E-01	6.43E-03
Chromium	4.00E-01	1.76E+01	4.40E+01	1.76E+01	4.40E+01
Copper	8.00E+01	3.98E+01	4.98E-01	3.98E+01	4.98E-01
Lead	1.70E+03	4.30E+01	2.53E-02	3.98E+01	2.34E-02
Manganese	4.50E+02	2.59E+02	5.76E-01	1.85E+02	4.10E-01
Mercury	1.00E-01	1.50E+00	1.50E+01	1.18E+00	1.18E+01
Vanadium	NA	2.13E+01		1.83E+01	
Zinc	1.20E+02	5.60E+02	4.67E+00	4.33E+02	3.61E+00
Polynuclear Aromatic Hydrocarbons					
Total HMW PAHs	1.80E+01	5.87E+00	3.26E-01	4.34E+00	2.41E-01
Semivolatile Organic Compounds					
Acetophenone	NA	6.20E-02		6.20E-02	
Benzaldehyde	NA	6.60E-02		6.60E-02	
Bis(2-ethylhexyl)phthalate	2.00E+02	2.20E-01	1.10E-03	2.20E-01	1.10E-03
Carbazole	NA	1.90E-02		1.90E-02	
Volatile Organic Compounds					
2-Butanone	NA	1.40E-02		1.40E-02	
Isopropylbenzene	NA	3.30E-04		3.30E-04	
Trichloroflouromethane	NA	5.00E-04		4.40E-04	
Xylenes (m & p)	NA	3.50E-02		3.50E-02	
Xylenes (o)	NA	1.20E-02		1.20E-02	

EPC = Exposure point concentrations

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

mg/kg dry wt = Milligram per kilogram of dry weight

NA = Reference value not available

UCL = Upper confidence level

Table 13
Maximum Modeled Doses to Birds Compared to Avian Toxicity Reference Values for AOC-4

	Avian TRV		Maximum Case Scenario HQs Based on Comparison of Doses to NOAELs	Maximum Case Scenario HQs Based on Comparison of Doses to LOAELs
Chemical	NOAEL	LOAEL	Insectivorous Birds	Insectivorous Birds
Metals				
Barium	2.08E+01	4.17E+01	2.29E+00	1.14E+00
Cadmium	1.45E+00	2.00E+01	1.18E+00	8.58E-02
Chromium	2.66E+00	5.00E+00	9.80E-01	5.21E-01
Copper	4.05E+00	6.17E+01	1.01E+00	6.60E-02
Lead	1.63E+00	1.13E+01	2.90E+00	4.18E-01
Manganese	9.97E+02	NA	1.05E-02	
Mercury	4.50E-01	9.00E-01	3.40E-01	1.70E-01
Vanadium	3.44E-01	6.88E-01	1.36E+01	6.79E+00
Zinc	6.61E+01	1.31E+02	2.49E+00	1.26E+00
Polynuclear Aromatic Hydrocarbons				
Total HMW PAHs	3.37E+00	3.37E+01	1.28E-01	1.28E-02
Semivolatile Organic Compounds	<del>_</del>	•		
Acetophenone	NA	NA		
Benzaldehyde	NA	NA		
Bis(2-ethylhexyl)phthalate	1.10E+00	NA	4.92E-02	
Carbazole	NA	NA		
Volatile Organic Compounds				
2-Butanone	NA	NA		
Isopropylbenzene	NA	NA		
Trichloroflouromethane	NA	NA		
Xylenes (m & p)	NA	NA		
Xylenes (o)	NA	NA		
NOTE:				

HQ = Hazard Quotient

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

LOAEL = Low Observed Adverse Effect Levels

mg/kg-bw day = Milligram of food per kilogram of body weight per day

NOAEL = No Observed Adverse Effect Levels

TRV = Toxicity reference value

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Table 14
95% UCL Mean Modeled Doses to Birds Compared to Avian Toxicity Reference Values for AOC-4

	Avian TR\		95% UCL Mean Case Scenario HQs Based on Comparison of Doses to NOAELs	95% UCL Mean Case Scenario HQs Based on Comparison of Doses to LOAELs		
Chemical	NOAEL	LOAEL	Insectivorous Birds	Insectivorous Birds		
Metals						
Barium	2.08E+01	4.17E+01	1.51E+00	7.52E-01		
Cadmium	1.45E+00	2.00E+01	1.18E+00	8.58E-02		
Chromium	2.66E+00	5.00E+00	9.80E-01	5.21E-01		
Copper	4.05E+00	6.17E+01	1.01E+00	6.60E-02		
Lead	1.63E+00	1.13E+01	2.72E+00	3.92E-01		
Manganese	9.97E+02	NA	7.82E-03			
Mercury	4.50E-01	9.00E-01	3.15E-01	1.58E-01		
Vanadium	3.44E-01 6.61E+01	6.88E-01 1.31E+02	1.16E+01	5.82E+00		
Zinc	0.01E+01	1.51E+02	2.26E+00	1.14E+00		
Polynuclear Aromatic Hydrocarbons						
Total HMW PAHs	3.37E+00	3.37E+01	1.15E-01	1.15E-02		
Semivolatile Organic Compounds						
Acetophenone	NA	NA				
Benzaldehyde	NA	NA				
Bis(2-ethylhexyl)phthalate	1.10E+00	NA	4.92E-02			
Carbazole	NA	NA				
Volatile Organic Compounds						
2-Butanone	NA	NA				
Isopropylbenzene	NA	NA				
Trichloroflouromethane	NA	NA				
Xylenes (m & p)	NA	NA				
Xylenes (o)	NA	NA				

NOTE:

HMW PAH: High molecular weight polynuclear aromatic hydrocarbon

HQ: Hazard Quotient

LOAEL: Low Observed Adverse Effect Levels

mg/kg-bw day: miligram of food per kilogram of body weight per day

NOAEL: No Observed Adverse Effect Levels

TRV: Toxicity reference value UCL: Upper confidence level

Table 15
Maximum Modeled Doses to Mammals Compared to Mammalian Toxicity Reference Value for AOC-4

		malian TRVs /kg-bw day)	Maximum Case Scenario HQs Based on Comparison of Doses to NOAELs		
Chemical	NOAEL	LOAEL	Insectivorous Mammals	Insectivorous Mammals	
Metals	•			-	
Barium	5.18E+01	4.36E+02	7.02E-01	8.34E-02	
Cadmium	7.70E-01	1.00E+01	1.56E+00	1.20E-01	
Chromium	2.40E+00	1.31E+01	7.85E-01	1.43E-01	
Copper	5.60E+00	1.54E+01	5.34E-01	1.94E-01	
Lead	4.70E+00	8.00E+01	7.36E-01	4.32E-02	
Manganese	5.15E+01	2.84E+02	1.61E-01	2.91E-02	
Mercury	1.32E+01	NA	8.51E-03		
Vanadium	4.16E+00	8.31E+00	8.02E-01	4.01E-01	
Zinc	7.54E+01	3.20E+02	1.55E+00	3.65E-01	
Polynuclear Aromatic Hydrocarbons					
Total HMW PAHs	6.15E-01	3.07E+00	5.18E-01	1.04E-01	
Semivolatile Organic Compounds					
Acetophenone	1.60E+02	NA	6.79E-05		
Benzaldehyde	NA	NA			
Bis(2-ethylhexyl)phthalate	1.83E+01	1.83E+02	2.11E-03	2.11E-04	
Carbazole	NA	NA			
Volatile Organic Compounds					
2-Butanone	1.77E+03	4.57E+03	1.38E-06	5.36E-07	
Isopropylbenzene	NA	NA			
Trichloroflouromethane	NA	NA			
Xylenes (m & p)	NA	NA			
Xylenes (o)	NA	NA			

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

HQ = Hazard Quotient

LOAEL = Low Observed Adverse Effect Levels

mg/kg-bw day = Milligram of food per kilogram of body weight per day

NOAEL = No Observed Adverse Effect Levels

TRV = Toxicity Reference Value

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Table 16
95% UCL Mean Modeled Doses to Mammals Compared to Mammalian Toxicity Reference Values for AOC-4

	Mammali (mg/kg-		95% UCL Mean Case Scenario HQs Based on Comparison of Doses to NOAELs	95% UCL Mean Case Scenario HQs Based on Comparison of Doses to LOAELs		
Chemical	NOAEL	LOAEL	Insectivorous Mammals	Insectivorous Mammals		
Metals						
Barium	5.18E+01	4.36E+02	4.61E-01	5.48E-02		
Cadmium	7.70E-01	1.00E+01	1.56E+00	1.20E-01		
Chromium	2.40E+00	1.31E+01	7.85E-01	1.43E-01		
Copper	5.60E+00	1.54E+01	5.34E-01	1.94E-01		
Lead	4.70E+00	8.00E+01	6.90E-01	4.05E-02		
Manganese	5.15E+01	2.84E+02	1.19E-01	2.16E-02		
Mercury	1.32E+01	NA	7.83E-03			
Vanadium	4.16E+00	8.31E+00	6.88E-01	3.44E-01		
Zinc	7.54E+01	3.20E+02	1.40E+00	3.31E-01		
Polynuclear Aromatic Hydrocarbons						
Total HMW PAHs	6.15E-01	3.07E+00	4.66E-01	9.34E-02		
Semivolatile Organic Compounds						
Acetophenone	1.60E+02	NA	6.79E-05			
Benzaldehyde	NA	NA				
Bis(2-ethylhexyl)phthalate	1.83E+01	1.83E+02	2.11E-03	2.11E-04		
Carbazole	NA	NA				
Volatile Organic Compounds						
2-Butanone	1.77E+03	4.57E+03				
Isopropylbenzene	NA	NA				
Trichloroflouromethane	NA	NA				
Xylenes (m & p)	NA	NA				
Xylenes (o)	NA	NA				
NOTE:						

#### NOTE:

TRV = Toxicity Reference Value

mg/kg-bw day = Milligram of food per kilogram of body weight per day

UCL = Upper confidence level

HQ = Hazard Quotient

NOAEL = No Observed Adverse Effect Levels

LOAEL = Low Observed Adverse Effect Levels

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

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Table 17

Frequency of Detection and Exposure Point Concentrations in Comparison to Background Data for AOC-4

			Surface Soil			
Analyte	Frequency of Detections	Maximum Detected Concentration (mg/kg)	95% UCL Mean (mg/kg)	Background 95% UPL (mg/kg)	Exceeds Background 95% UPL (mg/kg)	
Metals						
Barium	7/7	8.09E+02	5.32E+02	1.19E+03	No	
Cadmium	2/7	9.00E-01	9.00E-01	6.80E-01	Yes	
Chromium	7/7	1.76E+01	1.76E+01	6.15E+01	No	
Copper	7/7	3.98E+01	3.98E+01	2.84E+01	Yes	
Lead	7/7	4.30E+01	3.98E+01	5.02E+01	No	
Manganese	7/7	2.59E+02	1.85E+02	3.27E+02	No	
Mercury	7/7	1.50E+00	1.18E+00	2.10E-02	Yes	
Vanadium	7/7	2.13E+01	1.83E+01	1.93E+01	Yes	
Zinc	7/7	5.60E+02	4.33E+02	3.63E+03	No	

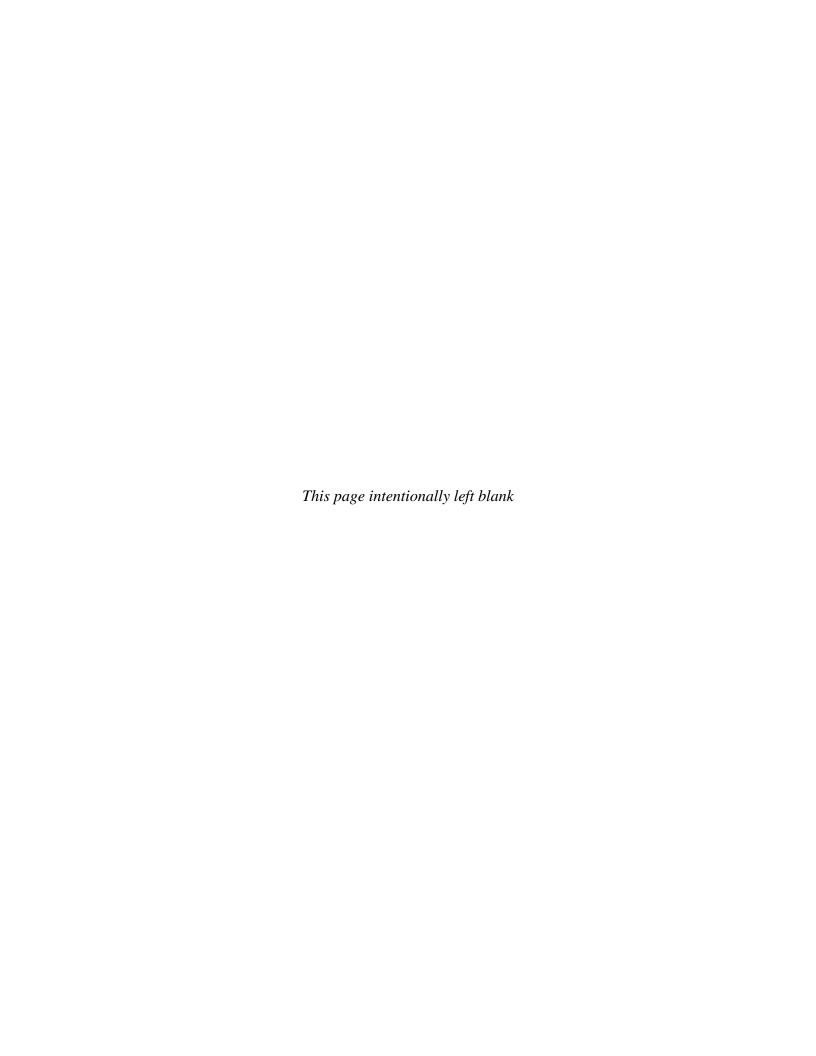
NOTE:

mg/kg = Milligram per kilogram

UCL = Upper confidence level

UPL = Upper prediction limit

# APPENDIX A AOC-4 DATA TABLES



# APPENDIX A-1 SURFACE SOIL DATA



TABLE A-1 SURFACE SOIL DATA

	Sample Name:	MW-17-0.0-0.5	SO4-01-0.0-0.5	SO4-01-0.0-0.5 Dup	SO4-02-0.0-0.5	SO4-03-0.0-0.5	SO4-04-0.0-0.5	SO4-04-0.0-0.5 Dup	SO4-05-0.0-0.5
Porce	nt Sample Name:	W1 W -1 7 - 0.0 - 0.3	304-01-0.0-0.3	SO4-01-0.0-0.5 Eup	504-02-0.0-0.5	304-03-0.0-0.3	304-04-0.0-0.3	SO4-04-0.0-0.5 Dap	504-05-0.0-0.5
1 ale	Sample Depth:	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5
	Date Sampled:	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013
Chemical Name	Unit	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013
INORGANICS	Cint								
Aluminum	mg/kg	2430	13300	17000	2000	2210	3930	3920	3450
Antimony	mg/kg	0.83 UJ	1 UJ	1.3 UJ	1.2 UJ	1.1 UJ	1.1 UJ	0.79 UJ	0.93 UJ
Arsenic	mg/kg	2	5.7	5.4	0.94	1.2	1.4	2	1.6 J
Barium	mg/kg	325	727	809	81.4	113	360	352	174
Beryllium	mg/kg	0.41 U	0.51 U	0.66 U	0.58 U	0.55 U	0.54 U	0.4 U	0.46 U
Cadmium	mg/kg	0.41 U	0.71	0.9	0.58 U	0.55 U	0.54 U	0.4 U	0.46 U
Calcium	mg/kg	180000	199000	184000	21700	264000	48300	56200	87700
Chromium	mg/kg	4.4 J	16.2 J	14.3 J	2	4.3	4.9 J	17.6 J	4 J
Cobalt	mg/kg	0.89	3.6	3.8	0.72	1.5	1.1	1.7	0.85 J
Copper	mg/kg	5.1	37.9	23.8	2.8	5.8	10.4	39.8	5 J
Iron	mg/kg	3770	11500	13000	2250 J	2620 J	4940	5160	7060
Lead	mg/kg	13.1	31.1	43	12.9	11.6	8.6	7.9	12.2
Magnesium	mg/kg	2470	5660	6010	1160	2370	1880	1860	1820
Manganese	mg/kg	108 J	259 J	250 J	65	137	89.7 J	97.8 J	106 J
Mercury	mg/kg	0.47	1.5	0.97	0.24	0.43	0.27	0.2	0.13
Nickel	mg/kg	2.6	18.5	11.1	1.7	2.3	3.1	13	2.6 J
Potassium	mg/kg	852	3340	4000	605	804	753	854	840
Selenium	mg/kg	2.1 U	2.5 U	3.3 U	2.9 U	2.7 U	2.7 U	2 U	2.3 U
Silver	mg/kg	0.41 U	0.51 U	0.66 U	0.58 U	0.55 U	0.54 U	0.4 U	0.46 U
Sodium	mg/kg	4230	1280	1460	449 U	2380	549	625	979
Thallium	mg/kg	0.41 U	0.51 U	0.66 U	0.58 U	0.55 U	0.54 U	0.4 U	0.46 U
Vanadium	mg/kg	5.5 J	17.5 J	21.3 J	3.4	6.5	6.8 J	4.7 J	5.1 J
Zinc	mg/kg	121	560	478	99.6	231	135	105	71.8
POLYNUCLEAR AROMATIC HYDROCARBONS			•		•	•	•		
2-Methylnaphthalene	ug/kg	36 U	46 U	22 U	7.7 U	57 U	73 U	74 U	72 U
Acenaphthene	ug/kg	21 LJ	46 U	22 U	5.1 LJ	57 U	73 U	32 LJ	72 U
Acenaphthylene	ug/kg	36 U	46 U	13 LJ	7.3 LJ	28 LJ	61 LJ	74 U	72 U
Anthracene	ug/kg	63	46 U	13 LJ	16	36 LJ	65 LJ	63 LJ	72 U
Benzo(a)anthracene	ug/kg	590	81	54	63	100	290	490	100
Benzo(a)pyrene	ug/kg	500	99	71	53	160	360	450	82
Benzo(b)fluoranthene	ug/kg	820	210	150	100	260	570	800	150
Benzo(g,h,i)perylene	ug/kg	210	66	52	22	150	200	210	34 LJ
Benzo(k)fluoranthene	ug/kg	220	55	43	28	72	160	270	43 LJ
Chrysene	ug/kg	600	120	90	70	190	290	520	100
Dibenz(a,h)anthracene	ug/kg	76	22 LJ	16 LJ	10	53 LJ	64 LJ	75	72 U
Fluoranthene	ug/kg	1400	180	98	160	250	430	950	210
Fluorene	ug/kg	15 LJ	46 U	22 U	3.7 LJ	57 U	73 U	74 U	72 U
Indeno(1,2,3-cd)pyrene	ug/kg	350	110	82	50	150	320	350	70 LJ
Naphthalene	ug/kg	36 U	46 U	22 U	7.7 U	57 U	73 U	74 U	72 U
Phenanthrene	ug/kg	350	43 LJ	26	49	89	170	230	92
Pyrene	ug/kg	1100	140	90	120	190	380	690	150
SEMIVOLATILE ORGANIC COMPOUNDS									
1,1-Biphenyl	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
1,2,4,5-Tetrachlorobenzene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,3,4,6-Tetrachlorophenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,4,5-Trichlorophenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,4,6-Trichlorophenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,4-Dichlorophenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,4-Dimethylphenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,4-Dinitrophenol	ug/kg	1800 U	2300 U	2200 U	770 U	1900 U	1800 U	1800 U	360 U

	Sample Name:	MW-17-0.0-0.5	SO4-01-0.0-0.5	SO4-01-0.0-0.5 Dup	SO4-02-0.0-0.5	SO4-03-0.0-0.5	SO4-04-0.0-0.5	SO4-04-0.0-0.5 Dup	SO4-05-0.0-0.5
	Parent Sample Name:	1111 17 0.0 0.5	504 01 0.0 0.5	SO4-01-0.0-0.5	504 02 0.0 0.5	504 03 0.0 0.3	50+ 0+ 0.0 0.5	SO4-04-0.0-0.5	504 05 0.0 0.5
	Sample Depth:	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5
	Date Sampled:	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013
Chemical Name	Unit	)/10/2013	y/10/2015	<i>y</i> /10/2015	J/10/2015	J/ 10/2015	y, 10, 2015	<i>7/10/2015</i>	y, 10, 2015
SEMIVOLATILE ORGANIC COMPOUNDS									
2.4-Dinitrotoluene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2,6-Dinitrotoluene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2-Chloronaphthalene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2-Chlorophenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2-Methylphenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
2-Nitroaniline	ug/kg	1800 U	2300 U	2200 U	770 U	1900 U	1800 U	1800 U	360 U
2-Nitrophenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
3,3-Dichlorobenzidine	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
3-Nitroaniline	ug/kg	1800 U	2300 U	2200 U	770 U	1900 U	1800 U	1800 U	360 U
4,6-Dinitro-2-methylphenol	ug/kg	1800 U	2300 U	2200 U	770 U	1900 U	1800 U	1800 U	360 U
4-Bromophenyl phenyl ether	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
4-Chloro-3-methylphenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
4-Chloroaniline	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
4-Chlorophenyl phenyl ether	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
4-Methylphenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
4-Nitroaniline	ug/kg	1800 U	2300 U	2200 U	770 U	1900 U	1800 U	1800 U	360 U
4-Nitrophenol	ug/kg	1800 U	2300 U	2200 U	770 U	1900 U	1800 U	1800 U	360 U
Acetophenone	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	62 LJ
Atrazine	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Benzaldehyde	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	66 LJ
Bis(2-chloroethoxy)methane	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Bis(2-chloroethyl)ether	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Bis(2-chloroisopropyl) ether	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Bis(2-ethylhexyl) phthalate	ug/kg	920 U	1200 U	1100 U	400 U	980 U	220 LJ	130 LJ	94 LJ
Butyl benzyl phthalate	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Caprolactum	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Carbazole	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	19 LJ
Dibenzofuran	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Diethyl phthalate	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Dimethyl phthalate	ug/kg	920 U	1200 U	1100 U	400 U	980 U	150 LJ	950 U	20 LJ
Di-n-butyl phthalate	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Di-n-octyl phthalate	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Hexachlorobenzene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Hexachlorobutadiene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Hexachlorocyclopentadiene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Hexachloroethane	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Isophorone	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Nitrobenzene	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
N-Nitrosodi-n-propylamine	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
N-Nitrosodiphenylamine	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	190 U
Pentachlorophenol	ug/kg	73 U	94 U	45 U	16 U	120 U	150 U	150 U	150 U
Phenol	ug/kg	920 U	1200 U	1100 U	400 U	980 U	940 U	950 U	33 LJ
VOLATILE ORGANIC COMPOUNDS									
1,1,1-Trichloroethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,1,2,2-Tetrachloroethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,1,2-Trichloro-1,2,2-trifluoroethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,1,2-Trichloroethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,1-Dichloroethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,1-Dichloroethene	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2,3-Trichlorobenzene	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2,4-Trichlorobenzene	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2-Dibromo-3-chloropropane (DBCP)	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2-Dibromoethane (Ethylene dibromide [EDB])	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U

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8	ample Name:	MW-17-0.0-0.5	SO4-01-0.0-0.5	SO4-01-0.0-0.5 Dup	SO4-02-0.0-0.5	SO4-03-0.0-0.5	SO4-04-0.0-0.5	SO4-04-0.0-0.5 Dup	SO4-05-0.0-0.5
	Parent Sample Name:		50+ 01 0.0 0.5	SO4-01-0.0-0.5	504 02 0.0 0.5	504 05 0.0 0.5	504 04 0.0 0.5	SO4-04-0.0-0.5	504 05 0.0 0.5
	ample Depth:	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5
	ate Sampled:	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013	9/10/2013
Chemical Name	Unit	2,20,202	2,20,202	.,	2,20,202	27.207.2020	77.207.2020	7,20,202	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
VOLATILE ORGANIC COMPOUNDS									
1,2-Dichlorobenzene	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1.2-Dichloroethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2-Dichloroethene (cis)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2-Dichloroethene (trans)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,2-Dichloropropane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,3-Dichlorobenzene	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,3-Dichloropropene (cis)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,3-Dichloropropene (trans)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,4-Dichlorobenzene	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
1,4-Dioxane	ug/kg	110 UJv	160 UJv	170 UJv	100 UJV	97 UJV	120 UJv	120 UJv	110 UJv
2-Butanone (Methyl ethyl ketone)	ug/kg	11 U	14 LJ	17 U	10 U	9.7 U	12 U	12 U	11 U
2-Hexanone	ug/kg	11 U	16 U	17 U	10 U	9.7 U	12 U	12 U	11 U
4-Methyl-2-pentanone (Methyl isobutyl ketone [MIBK])	ug/kg	11 U	16 U	17 U	10 U	9.7 U	12 U	12 U	11 U
Acetone	ug/kg	11 U	16 U	17 U	10 U	9.7 U	12 U	12 U	11 U
Benzene	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Bromochloromethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Bromodichloromethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Bromoform	ug/kg	5.3 U	R	R	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Bromomethane (Methyl bromide)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Carbon disulfide	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Carbon tetrachloride	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Chlorobenzene	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Chloroethane (Ethyl chloride)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Chloroform	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Chloromethane (Methyl chloride)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Cyclohexane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Dibromochloromethane (Chlorodibromomethane)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Dichlorodifluoromethane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Ethylbenzene	ug/kg	5.3 U	3.7 LJ	1.6 LJ	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Isopropylbenzene (Cumene)	ug/kg	5.3 U	0.33 LJ	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
m- & p-Xylenes	ug/kg	0.15 LJ	35 J	14	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Methyl acetate	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Methylcyclohexane	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Methylene chloride	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Methyl-tertiary-butyl ether (MtBE)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
o-Xylene	ug/kg	5.3 U	12	4.2 LJ	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Styrene	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Tetrachloroethene (PCE)	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Toluene	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Trichloroethene (TCE)	ug/kg	5.3 U	1.2 LJ	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
Trichlorofluoromethane	ug/kg	0.25 LJ	0.5 LJ	0.48 LJ	5.1 U	4.9 U	0.27 LJ	0.18 LJ	0.23 LJ
Vinyl chloride	ug/kg	5.3 U	7.9 U	8.7 U	5.1 U	4.9 U	5.9 U	5.9 U	5.6 U
NOTE:		Qualifiers:						<u> </u>	
mg/kg = Milligram per kilogram		J = Indicates an est							
ug/kg = Microgram per kilogram		L = Result is biase	d low						
		R = Result is unusa	able						
		U = Not detected							

# APPENDIX A-2 SURFACE SOIL BACKGROUND DATA

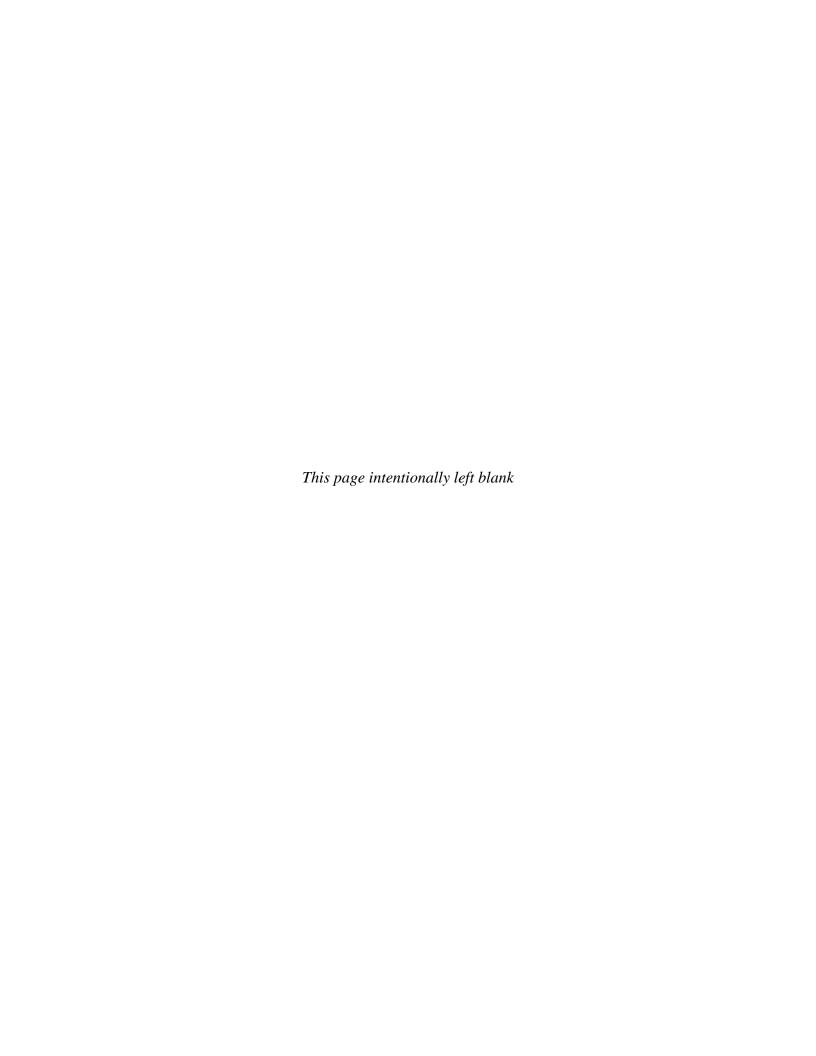


TABLE A-2.
SURFACE SOIL BACKGROUND DATA

Sa	mple Name:	FR-252	FR-253	FR-255	FR-259	FR-262	TWB-01-0.0-0.5	TWB-02-0.0-0.5	TWB-03-0.0-0.5	TWB-03-0.0-0.5 Dup	TWB-04-0.0-0.5
Parent Sa	mple Name:									TWB-03-0.0-0.5	
Sa	mple Depth:						0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5
Da	te Sampled:	1/16/2008	1/16/2008	1/16/2008	1/16/2008	1/16/2008	9/13/2013	9/13/2013	9/13/2013	9/13/2013	9/13/2013
Chemical Name	Unit										
INORGANICS											
Aluminum	mg/kg	2280	2230	918	762	10500	6480	3700	2780	2530	1630
Antimony	mg/kg	0.84 B	0.75 B	NR	NR	NR	1.7 J	0.87 UJ	0.8 UJ	1 UJ	1 UJ
Arsenic	mg/kg	NR	0.33 B	NR	0.29 B	2.8	4.6 J-	0.66 J-	0.89 J-	0.97 J-	1.3
Barium	mg/kg	33	38.5	19.6 B	43	1520	543 J	346 J	228 J	230 J	169
Beryllium	mg/kg	0.093 B	0.075 B	NR	NR	0.44 B	0.59 U	0.43 U	0.4 U	0.5 U	0.5 U
Cadmium	mg/kg	NR	NR	NR	NR	0.68	0.59 U	0.43 U	0.4 U	0.5 U	0.5 U
Calcium	mg/kg	252000	195000	8540	835	110000	85700	33900	41800	32000	212000
Chromium	mg/kg	4.5	4.1	0.9 B	0.94 B	92.3	12	4.8	5.2	5.7	38.9 J
Chromium, hexavalent	mg/kg	NR	NR	NR	NR	2.1 B	NR	NR	NR	NR	NR
Cobalt	mg/kg	0.73 B	0.44 B	NR	NR	4.8 B	2.1	0.89	0.86	0.91	1.2
Copper	mg/kg	4.8	5.4	0.92 B	4.2	16.6	39.9 J	5.9 J	7.5 J	7.5 J	11.3
Iron	mg/kg	1610	1550	604	625	34500	10500	3460	8920	3430	4180
Lead	mg/kg	5.1	5.7	5	4	19.6	27.3	23.3	30.6	32.3	27.4
Magnesium	mg/kg	1220	1000	199 B	105 B	5140	2410	1010	1030	870	1620
Manganese	mg/kg	74.5	55.9	35.4	18.1	345	219	114	133	102	145
Mercury	mg/kg	0.012 B	0.01 B	0.0065 B	0.0044 B	0.0062 B	0.025 LJ	0.015 LJ	0.012 LJ	0.01 LJ	0.012 LJ
Nickel	mg/kg	3.4 B	2.6 B	0.44 B	0.3 B	7.8	6.9	4.4	3.2	3.4	5.1 J
Potassium	mg/kg	647	616	130 B	183 B	2500	1020	696	509	453	384 U
Selenium	mg/kg	1.3	1.3	NR	NR	1 B	2.9 U	2.2 U	2 U	2.5 U	2.5 U
Silver	mg/kg	NR	NR	NR	NR	0.11 B	0.59 U	0.43 U	0.4 U	0.5 U	0.5 U
Sodium	mg/kg	35 B	48.6 B	NR	NR	1280	490 U	540 U	427 U	432 U	384 U
Thallium	mg/kg	NR	NR	NR	NR	NR	0.59 U	0.43 U	0.4 U	0.5 U	0.5 U
Vanadium	mg/kg	6.6	5.8	1.2 B	0.93 B	23.7	13.9	4.9	5.2	5.7	2.9 J
Zinc	mg/kg	41.3	48.1	9.2	18.2	3630	203 J	54.8 J	71.5 J	68.6 J	101
NOTE:			Qualifiers:	·	·		-				

mg/kg = milligram(s) per kilogram

Qualifiers:

U = Not detected

J = Indicates an estimated value

L = Result is biased low

 $R = Result \ is \ unusable$ 

NR = No result

TABLE A-2.
SURFACE SOIL BACKGROUND DATA

Sa	ample Name:	TWB-05-0.0-0.5	TWB-06-0.0-0.5	TWB-06-0.0-0.5 Dup	TWB-07-0.0-0.5	TWB-08-0.0-0.5	TWB-09-0.0-0.5	TWB-09-0.0-0.5 Dup	TWB-10-0.0-0.5
	ample Name:			TWB-06-0.0-0.5				TWB-09-0.0-0.5	
Sa	imple Depth:	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5	0.0-0.5
	ate Sampled:	9/13/2013	9/13/2013	9/13/2013	9/13/2013	9/14/2013	9/14/2013	9/14/2013	9/14/2013
Chemical Name	Unit								
INORGANICS									
Aluminum	mg/kg	2140	4790	3270	2740	1020	965	737	3580
Antimony	mg/kg	1 UJ	0.81 UJ	1.1 UJ	1.1 UJ	0.77 UJ	0.95 UJ	0.87 UJ	1.1 UJ
Arsenic	mg/kg	0.94 J-	1.3	1.4	0.53 U	0.42 J-	0.48 UJ	0.44 UJ	1.3 J-
Barium	mg/kg	115 J	1070	1020	20.6	26.8 J	25.5 J	28.9 J	169 J
Beryllium	mg/kg	0.52 U	0.4 U	0.54 U	0.53 U	0.39 U	0.48 U	0.44 U	0.56 U
Cadmium	mg/kg	0.52 U	0.4 U	0.54 U	0.53 U	0.39 U	0.48 U	0.44 U	0.56 U
Calcium	mg/kg	69600	653000	129000	10900	6740	19700	187000	100000
Chromium	mg/kg	5.1	25.1 J	15 J	1.5 J	4.1	1.1	1.7	6.2
Chromium, hexavalent	mg/kg	NR	NR	NR	NR	NR	NR	NR	NR
Cobalt	mg/kg	0.83	1.8	1.7	0.53 U	0.39 U	0.48 U	0.44 U	1.1
Copper	mg/kg	6.5 J	12.4	13.8	3.3	2.5 J	1.8 J	2.5 J	13.6 J
Iron	mg/kg	5570	6550	7660	2020	929	987	708	4170
Lead	mg/kg	22.4	30.2	48	5	6.5	9.4	10.7	19.1
Magnesium	mg/kg	1410	1870	1930	471 LJ	292 LJ	378 LJ	650	1450
Manganese	mg/kg	107	190	183	31.9	17	23.6	32.7	93.4
Mercury	mg/kg	0.014 LJ	0.011 LJ	0.0098 LJ	0.012 LJ	0.0065 LJ	0.0091 LJ	0.0073 LJ	0.0094 LJ
Nickel	mg/kg	3.5	13.4 J	7.6 J	0.91 J	1.2	1.3	1.2	4.4
Potassium	mg/kg	528 U	975	642	476 U	403 U	462 U	348 U	952
Selenium	mg/kg	2.6 U	2 U	2.7 U	2.7 U	1.9 U	2.4 U	2.2 U	2.8 U
Silver	mg/kg	0.52 U	0.4 U	0.54 U	0.53 U	0.39 U	0.48 U	0.44 U	0.56 U
Sodium	mg/kg	528 U	270 U	408 U	476 U	403 U	462 U	348 U	473 U
Thallium	mg/kg	0.52 U	0.4 U	0.54 U	0.53 U	0.39 U	0.48 U	0.44 U	0.56 U
Vanadium	mg/kg	5.9	7.2 J	7.9 J	1.8 LJ	2.8	6.3	2.3	8.6
Zinc	mg/kg	66.1 J	117	118	17.3	18.7 J	11.4 J	16.6 J	71 J
NOTE.		Ouglifican			-	-			

Qualifiers:

mg/kg = milligram(s) per kilogram U = Not detected

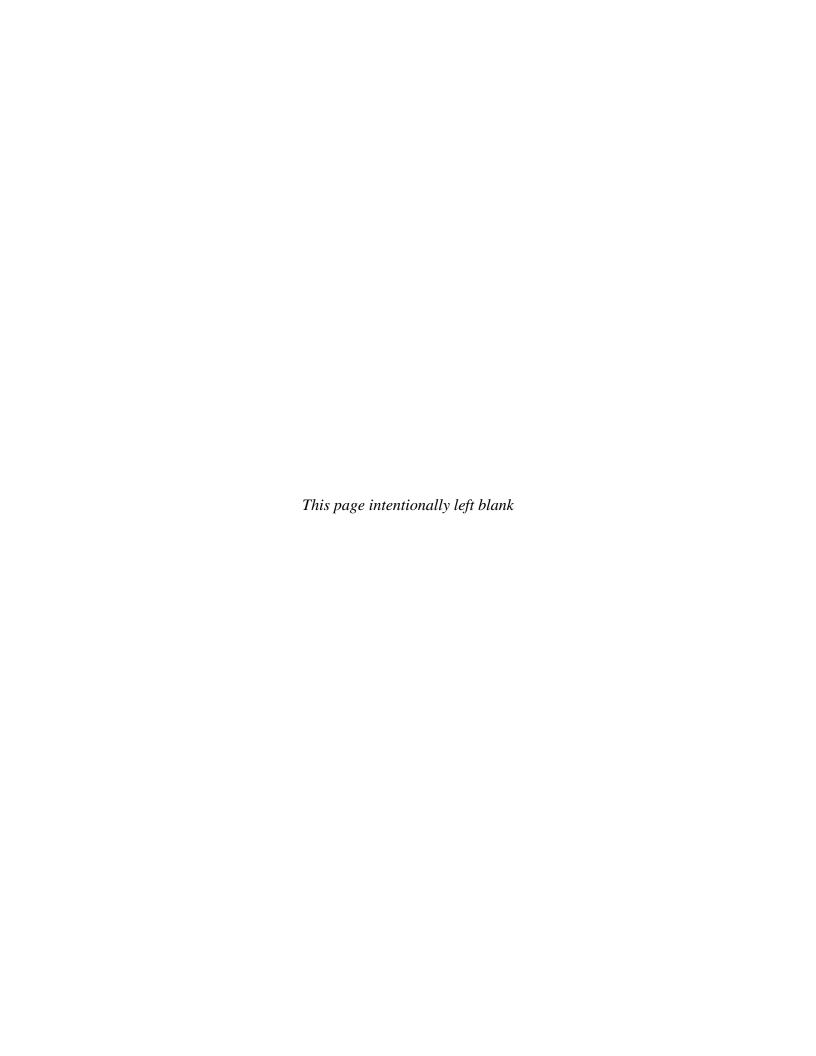
J = Indicates an estimated value L = Result is biased low

 $R = Result \ is \ unusable$ 

NR = No result

### **APPENDIX B**

**Food Web Calculations** 



#### Table B-1 Wildlife Exposure Modeling of Maximum Doses to Insectivorous Birds (American Robin) from Media for AOC-4

Exposure Parameters

Soil Ingestion Rate (kg dry wt./kg bw-day): 2.34E-02 kg/kg-day Food Ingestion Rate (kg dry wt./kg bw-day): 2.23E-01 kg/kg-day

		Food Item (Insect/Wo	Maximum Case Scenario Doses			
Chemical	Maximum Soil Concentration (mg/kg dry wt.)	BAF/Equation (mg/kg dry wt. to mg/kg dry wt.)	Maximum Food Item Tissue Concentration (mg/kg dry wt.)	Dose from Soil (mg/kg bw-day)	Dose from Food (mg/kg bw-day)	Total Dose (mg/kg bw-day)
Metals						
Barium	8.09E+02	1.60E-01	1.29E+02	1.89E+01	2.88E+01	4.77E+01
Cadmium	9.00E-01	ln(dry worm conc, mg/kg) = (2.114+0.795*ln(soil conc))	7.62E+00	2.10E-02	1.69E+00	1.72E+00
Chromium	1.76E+01	ln(dry worm conc, mg/kg) = (2.481+-0.067*ln(soil conc))	9.86E+00	4.11E-01	2.19E+00	2.61E+00
Copper	3.98E+01	ln(dry worm conc, mg/kg) = (1.675+0.264*ln(soil conc))	1.41E+01	9.30E-01	3.14E+00	4.07E+00
Lead	4.30E+01	ln(dry worm conc, mg/kg) = (-0.218+0.807*ln(soil conc))	1.67E+01	1.00E+00	3.72E+00	4.73E+00
Manganese	2.59E+02	ln(dry worm conc, mg/kg) = (-0.809+0.682*ln(soil conc))	1.97E+01	6.05E+00	4.38E+00	1.04E+01
Mercury	1.50E+00	ln(dry worm conc, mg/kg) = (-0.684+0.118*ln(soil conc))	5.29E-01	3.50E-02	1.18E-01	1.53E-01
Vanadium	2.13E+01	8.80E-01	1.87E+01	4.98E-01	4.17E+00	4.67E+00
Zinc	5.60E+02	ln(dry worm conc, mg/kg) = (4.449+0.328*ln(soil conc))	6.82E+02	1.31E+01	1.52E+02	1.65E+02
Polynuclear Aromatic Hydrocarbons						
Total HMW PAHs	5.87E+00		1.47E+00	1.06E-01	3.27E-01	4.33E-01
Semivolatile Organic Compounds						
Acetophenone	6.20E-02	1.00E+00	6.20E-02	1.45E-03	1.38E-02	1.52E-02
Benzaldehyde	6.60E-02	1.00E+00	6.60E-02	1.54E-03	1.47E-02	1.62E-02
Bis(2-ethylhexyl)phthalate	2.20E-01	1.00E+00	2.20E-01	5.14E-03	4.90E-02	5.41E-02
Carbazole	1.90E-02	1.00E+00	1.90E-02	4.44E-04	4.23E-03	4.67E-03
Volatile Organic Compounds						
2-Butanone	1.40E-02	1.00E+00	1.40E-02	3.27E-04	3.12E-03	3.44E-03
Trichloroflouromethane	5.00E-04	1.00E+00	5.00E-04	1.17E-05	1.11E-04	1.23E-04
Xylenes (m & p)	3.50E-02	1.00E+00	3.50E-02	8.18E-04	7.79E-03	8.61E-03
Xylenes (o)	1.20E-02	1.00E+00	1.20E-02	2.80E-04	2.67E-03	2.95E-03
NOTE:						

NOTE:

 $BAF = Bioaccululation \ Factor$ 

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

kg = Kilogran

L/kg bw-day = Liters per kilogram of body weight per day

mg/kg bw-day = Milligram of food per kilogram of body weight per day

mg/kg dry wt. = Milligram per kilogram of dry weight

 $mg/L = Milligram \ per \ liter$ 

#### Table B-2 Wildlife Exposure Modeling of 95% UCL Mean Doses to Insectivorous Birds (American Robin) from Media for AOC-4

**Exposure Parameters** 

Soil Ingestion Rate (kg dry wt./kg bw-day): 2.34E-02 kg/kg-day Food Ingestion Rate (kg dry wt./kg bw-day): 2.23E-01 kg/kg-day

		Food Item (Insect/Worm) Uptake		95% UCL Mean Case Scenario Doses			
Chemical	95% UCL Mean Soil Concentration (mg/kg dry wt.)	BAF/Equation (mg/kg dry wt. to mg/kg dry wt.)	95% UCL Mean Food Item Tissue Concentration (mg/kg dry wt.)	Dose from Soil	Dose from Food (mg/kg bw-day)	Total Dose (mg/kg bw-day)	
Metals	* ( <del></del>			• 0 0			
Barium	5.32E+02	1.60E-01	8.50E+01	1.24E+01	1.89E+01	3.13E+01	
Cadmium	9.00E-01	ln(dry worm conc, mg/kg) = (2.114+0.795*ln(soil conc))	7.62E+00	2.10E-02	1.69E+00	1.72E+00	
Chromium	1.76E+01	ln(dry worm conc, mg/kg) = (2.481+-0.067*ln(soil conc))		4.11E-01	2.19E+00	2.61E+00	
Copper	3.98E+01	ln(dry worm conc, mg/kg) = (1.675+0.264*ln(soil conc))	1.41E+01	9.30E-01	3.14E+00	4.07E+00	
Lead	3.98E+01	ln(dry worm conc, mg/kg) = (-0.218+0.807*ln(soil conc))	1.57E+01	9.31E-01	3.50E+00	4.43E+00	
Manganese	1.85E+02	ln(dry worm conc, mg/kg) = (-0.809+0.682*ln(soil conc))	1.56E+01	4.31E+00	3.48E+00	7.79E+00	
Mercury	1.18E+00	ln(dry worm conc, mg/kg) = (-0.684+0.118*ln(soil conc))	5.14E-01	2.75E-02	1.14E-01	1.42E-01	
Vanadium	1.83E+01	8.80E-01	1.61E+01	4.27E-01	3.58E+00	4.01E+00	
Zinc	4.33E+02	ln(dry worm conc, mg/kg) = (4.449+0.328*ln(soil conc))	6.27E+02	1.01E+01	1.39E+02	1.50E+02	
Polynuclear Aromatic Hydrocarbons							
Total HMW PAHs	4.34E+00		1.32E+00	9.59E-02	2.93E-01	3.89E-01	
Semivolatile Organic Compounds							
Acetophenone	6.20E-02	1.00E+00	6.20E-02	1.45E-03	1.38E-02	1.52E-02	
Benzaldehyde	6.60E-02	1.00E+00	6.60E-02	1.54E-03	1.47E-02	1.62E-02	
Bis(2-ethylhexyl)phthalate	2.20E-01	1.00E+00	2.20E-01	5.14E-03	4.90E-02	5.41E-02	
Carbazole	1.90E-02	1.00E+00	1.90E-02	4.44E-04	4.23E-03	4.67E-03	
Volatile Organic Compounds							
2-Butanone	1.40E-02	1.00E+00	1.40E-02	3.27E-04	3.12E-03	3.44E-03	
Trichloroflouromethane	4.40E-04	1.00E+00	4.40E-04	1.03E-05	9.78E-05	1.08E-04	
Xylenes (m & p)	3.50E-02	1.00E+00	3.50E-02	8.18E-04	7.79E-03	8.61E-03	
Xylenes (o)	1.20E-02	1.00E+00	1.20E-02	2.80E-04	2.67E-03	2.95E-03	

#### NOTE:

 $BAF = Bioaccululation \ Factor$ 

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

kg=Kilogram

L/kg bw-day = Liters per kilogram of body weight per day

mg/kg bw-day = Milligram of food per kilogram of body weight per day

mg/kg dry wt. = Milligram per kilogram of dry weight

mg/L = Milligram per liter

UCL = Upper confidence level

Table B-3
Wildlife Exposure Modeling of Maximum Doses to Insectivorous Mammals (Northern Short-Tailed Shrew) from Media for AOC-4

**Exposure Parameters** 

Soil Ingestion Rate (kg dry wt./kg bw-day): 2.02E-02 kg/kg-day Food Ingestion Rate (kg dry wt./kg bw-day): 1.55E-01 kg/kg-day

		Food Item (Insect/Wo	Mavir	num Case Scenario	Doses	
Chemical	Maximum Soil Concentration (mg/kg dry wt.)	BAF/Equation (mg/kg dry wt. to mg/kg dry wt.)	Maximum Food Item Tissue Concentration (mg/kg dry wt.)	Dose from Soil (mg/kg bw-day)	Dose from Food (mg/kg bw-day)	Total Dose (mg/kg bw-day)
Metals						
Barium	8.09E+02	1.60E-01	1.29E+02	1.63E+01	2.01E+01	3.64E+01
Cadmium	9.00E-01	ln(dry worm conc, mg/kg) = (2.114+0.795*ln(soil conc))	7.62E+00	1.81E-02	1.18E+00	1.20E+00
Chromium	1.76E+01	ln(dry worm conc, mg/kg) = (2.481+-0.067*ln(soil conc))	9.86E+00	3.55E-01	1.53E+00	1.88E+00
Copper	3.98E+01	$\begin{aligned} &\ln(\text{dry worm conc, mg/kg}) = \\ &(1.675 + 0.264 * \ln(\text{soil conc})) \end{aligned}$	1.41E+01	8.02E-01	2.19E+00	2.99E+00
Lead	4.30E+01	ln(dry worm conc, mg/kg) = (-0.218+0.807*ln(soil conc))	1.67E+01	8.66E-01	2.59E+00	3.46E+00
Manganese	2.59E+02	ln(dry worm conc, mg/kg) = (-0.809+0.682*ln(soil conc))	1.97E+01	5.22E+00	3.05E+00	8.27E+00
Mercury	1.50E+00	ln(dry worm conc, mg/kg) = (-0.684+0.118*ln(soil conc))	5.29E-01	3.02E-02	8.20E-02	1.12E-01
Vanadium	2.13E+01	8.80E-01	1.87E+01	4.29E-01	2.91E+00	3.33E+00
Zinc	5.60E+02	ln(dry worm conc, mg/kg) = (4.449+0.328*ln(soil conc))	6.82E+02	1.13E+01	1.06E+02	1.17E+02
Polynuclear Aromatic Hydrocarbons						
Total HMW PAHs	5.87E+00		1.47E+00	9.14E-02	2.28E-01	3.19E-01
Semivolatile Organic Compounds						
Acetophenone	6.20E-02	1.00E+00	6.20E-02	1.25E-03	9.61E-03	1.09E-02
Benzaldehyde	6.60E-02	1.00E+00	6.60E-02	1.33E-03	1.02E-02	1.16E-02
Bis(2-ethylhexyl)phthalate	2.20E-01	1.00E+00	2.20E-01	4.43E-03	3.41E-02	3.85E-02
Carbazole	1.90E-02	1.00E+00	1.90E-02	3.83E-04	2.95E-03	3.33E-03
Volatile Organic Compounds						
2-Butanone	1.40E-02	1.00E+00	1.40E-02	2.82E-04	2.17E-03	2.45E-03
Trichloroflouromethane	5.00E-04	1.00E+00	5.00E-04	1.01E-05	7.75E-05	8.76E-05
Xylenes (m & p)	3.50E-02	1.00E+00	3.50E-02	7.05E-04	5.43E-03	6.13E-03
Xylenes (o)	1.20E-02	1.00E+00	1.20E-02	2.42E-04	1.86E-03	2.10E-03

#### NOTE:

BAF = Bioaccululation Factor

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

kg=Kilogram

L/kg bw-day = Liters per kilogram of body weight per day

mg/kg bw-day = Milligram of food per kilogram of body weight per day

 $mg/kg \; dry \; wt. = Milligram \; per \; kilogram \; of \; dry \; weight$ 

mg/L = Milligram per liter

Table B-4
Wildlife Exposure Modeling of 95% UCL Mean Doses to Insectivorous Mammals (Northern Short-Tailed Shrew) from Media for AOC-4

**Exposure Parameters** 

Soil Ingestion Rate (kg dry wt./kg bw-day): 2.02E-02 kg/kg-day Food Ingestion Rate (kg dry wt./kg bw-day): 1.55E-01 kg/kg-day

		Food Item (Insect/Worm) Uptake		95% UCL Mean Case Scenario Doses			
Chemical	95% UCL Mean Soil Concentration (mg/kg dry wt.)	BAF/Equation (mg/kg dry wt. to mg/kg dry wt.)	95% UCL Mean Food Item Tissue Concentration (mg/kg dry wt.)	Dose from Soil	Dose from Food (mg/kg bw-day)	Total Dose (mg/kg bw-day)	
Metals	(mg/kg ary wt.)	mg/kg dry wt.)	(mg/kg dry wt.)	(mg/kg bw-day)	(mg/kg bw-day)	(IIIg/Kg DW-day)	
Barium	5.32E+02	1.60E-01	8.50E+01	1.07E+01	1.32E+01	2.39E+01	
Cadmium	9.00E-01	ln(dry worm conc, mg/kg) = (2.114+0.795*ln(soil conc))	7.62E+00	1.81E-02	1.18E+00	1.20E+00	
Chromium	1.76E+01	ln(dry worm conc, mg/kg) = (2.481+-0.067*ln(soil conc))	9.86E+00	3.55E-01	1.53E+00	1.88E+00	
Copper	3.98E+01	ln(dry worm conc, mg/kg) = (1.675+0.264*ln(soil conc))	1.41E+01	8.02E-01	2.19E+00	2.99E+00	
Lead	3.98E+01	ln(dry worm conc, mg/kg) = (-0.218+0.807*ln(soil conc))	1.57E+01	8.03E-01	2.44E+00	3.24E+00	
Manganese	1.85E+02	ln(dry worm conc, mg/kg) = (-0.809+0.682*ln(soil conc))	1.56E+01	3.72E+00	2.42E+00	6.14E+00	
Mercury	1.18E+00	ln(dry worm conc, mg/kg) = (-0.684+0.118*ln(soil conc))	5.14E-01	2.37E-02	7.97E-02	1.03E-01	
Vanadium	1.83E+01	8.80E-01	1.61E+01	3.68E-01	2.49E+00	2.86E+00	
Zinc	4.33E+02	ln(dry worm conc, mg/kg) = (4.449+0.328*ln(soil conc))	6.27E+02	8.72E+00	9.71E+01	1.06E+02	
Polynuclear Aromatic Hydrocarbons							
Total HMW PAHs	4.34E+00		1.32E+00	8.27E-02	2.04E-01	2.87E-01	
Semivolatile Organic Compounds							
Acetophenone	6.20E-02	1.00E+00	6.20E-02	1.25E-03	9.61E-03	1.09E-02	
Benzaldehyde	6.60E-02	1.00E+00	6.60E-02	1.33E-03	1.02E-02	1.16E-02	
Bis(2-ethylhexyl)phthalate	2.20E-01	1.00E+00	2.20E-01	4.43E-03	3.41E-02	3.85E-02	
Carbazole	1.90E-02	1.00E+00	1.90E-02	3.83E-04	2.95E-03	3.33E-03	
Volatile Organic Compounds							
2-Butanone	1.40E-02	1.00E+00	1.40E-02	2.82E-04	2.17E-03	2.45E-03	
Trichloroflouromethane	4.40E-04	1.00E+00	4.40E-04	8.86E-06	6.81E-05	7.70E-05	
Xylenes (m & p)	3.50E-02	1.00E+00	3.50E-02	7.05E-04	5.43E-03	6.13E-03	
Xylenes (o)	1.20E-02	1.00E+00	1.20E-02	2.42E-04	1.86E-03	2.10E-03	
NOTE			_				

NOTE:

 $BAF = Bioaccululation \ Factor$ 

HMW PAH = High molecular weight polynuclear aromatic hydrocarbon

kg = Kilogram

L/kg bw-day = Liters per kilogram of body weight per day

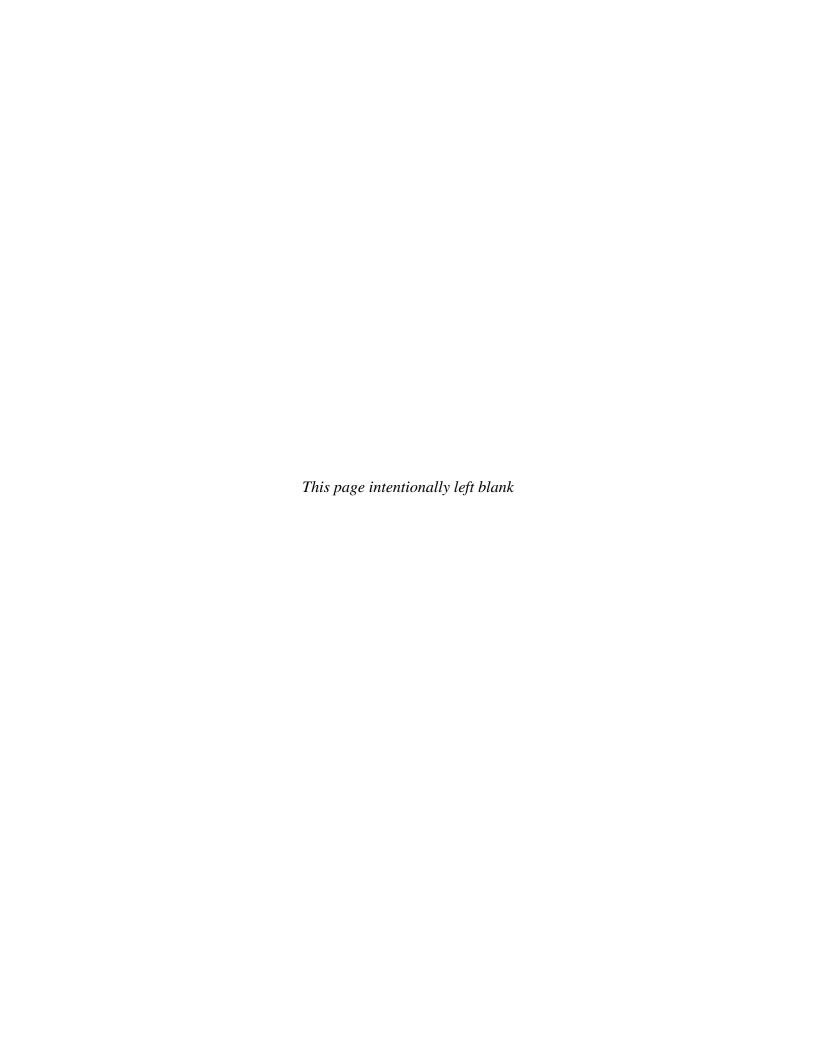
mg/kg bw-day = Milligram of food per kilogram of body weight per day

 $mg/kg \ dry \ wt. = Milligram \ per \ kilogram \ of \ dry \ weight$ 

mg/L = Milligram per liter

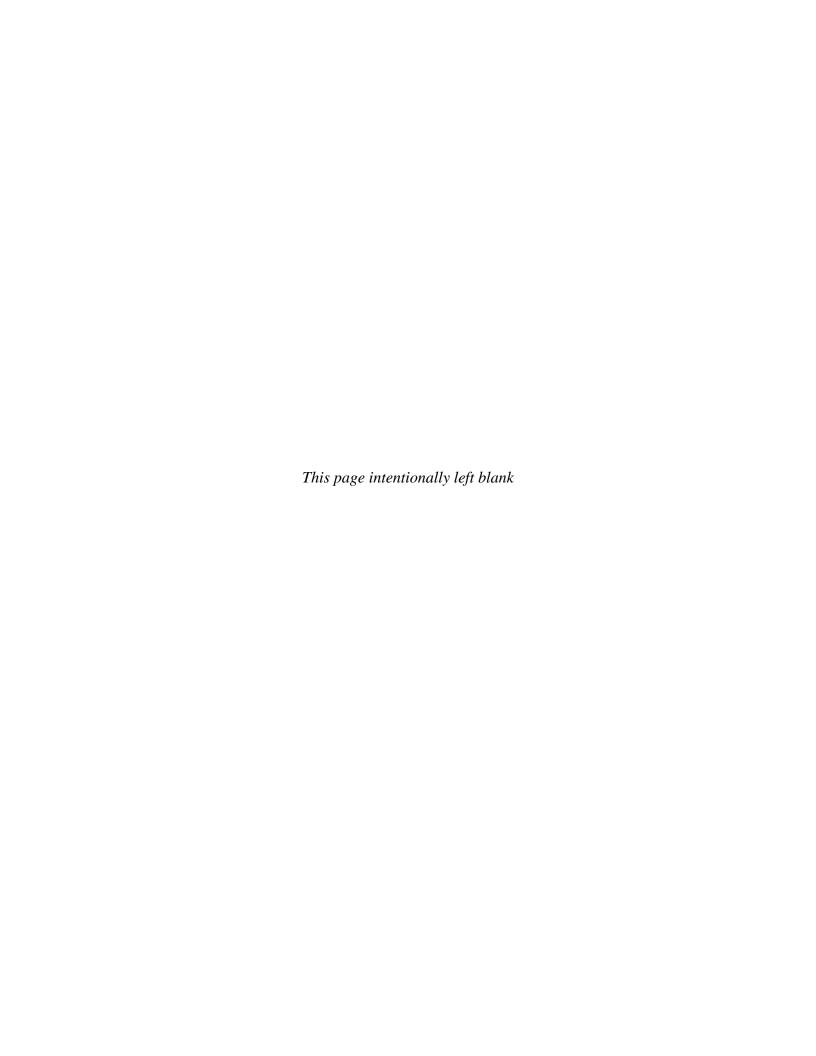
UCL: Upper confidence level

# APPENDIX C ProUCL STATISTICAL DATA OUTPUT



### **APPENDIX C-1**

# ProUCL STATISTICAL DATA OUTPUT – ALL FIELD DATA



#### User Selected Options

| From File | Sheet1.wst | Full Precision | OFF | Confidence Coefficient | 95% | Number of Bootstrap Operations | 10000 |

#### SS\_Acenaphthylene

	General S	tatistics	
Number of Valid Data	6	Number of Detected Data	4
Number of Distinct Detected Data	4	Number of Non-Detect Data	2
		Percent Non-Detects	33.33%
Raw Statistics		Log-transformed Statistics	
Minimum Detected	0.0073	Minimum Detected	-4.92
Maximum Detected	0.061	Maximum Detected	-2.797
Mean of Detected	0.0273	Mean of Detected	-3.909
SD of Detected	0.0241	SD of Detected	0.923
Minimum Non-Detect	0.036	Minimum Non-Detect	-3.324
Maximum Non-Detect	0.072	Maximum Non-Detect	-2.631
Note: Data have multiple DLs - Use of KM Method is recommen	ded	Number treated as Non-Detect	6
For all methods (except KM, DL/2, and ROS Methods),		Number treated as Detected	0
Observations < Largest ND are treated as NDs		Single DL Non-Detect Percentage	100.00%

Warning: There are only 4 Distinct Detected Values in this data

Note: It should be noted that even though bootstrap may be performed on this data set

the resulting calculations may not be reliable enough to draw conclusions

It is recommended to have 10-15 or more distinct observations for accurate and meaningful results.

	UCL Statis	tice	
Normal Distribution Test with Detected Values Only		Lognormal Distribution Test with Detected Values On	ly
Shapiro Wilk Test Statistic	0.893	Shapiro Wilk Test Statistic	0.985
5% Shapiro Wilk Critical Value	0.748	5% Shapiro Wilk Critical Value	0.748
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level	
Assuming Normal Distribution		Assuming Lognormal Distribution	
DL/2 Substitution Method		DL/2 Substitution Method	
Mean	0.0272	Mean	-3.829
SD	0.0195	SD	0.758
95% DL/2 (t) UCL	0.0433	95% H-Stat (DL/2) UCL	0.09
Maximum Likelihood Estimate(MLE) Method	N/A	Log ROS Method	
MLE method failed to converge properly		Mean in Log Scale	-3.989
		SD in Log Scale	0.731
		Mean in Original Scale	0.0235
		SD in Original Scale	0.0196
		95% t UCL	0.0397
		95% Percentile Bootstrap UCL	0.037
		95% BCA Bootstrap UCL	0.0411
		95% H-UCL	0.0702
Gamma Distribution Test with Detected Values Only	•	Data Distribution Test with Detected Values Only	
k star (bias corrected)	0.609	Data appear Normal at 5% Significance Level	
Theta Star	0.0449		
nu star	4.868		
A-D Test Statistic	0.243	Nonparametric Statistics	
5% A-D Critical Value	0.661	Kaplan-Meier (KM) Method	
K-S Test Statistic	0.661	Mean	0.0251
5% K-S Critical Value	0.399	SD	0.0196
Data appear Gamma Distributed at 5% Significance Le	evel	SE of Mean	0.0104
		95% KM (t) UCL	0.046
Assuming Gamma Distribution		95% KM (z) UCL	0.0421
Gamma ROS Statistics using Extrapolated Data		95% KM (jackknife) UCL	0.0463
Minimum	0.0073	95% KM (bootstrap t) UCL	0.0635
Maximum	0.061	95% KM (BCA) UCL	0.0431
Mean	0.0244	95% KM (Percentile Bootstrap) UCL	0.0431
Median	0.0186	95% KM (Chebyshev) UCL	0.0703
SD	0.0193	97.5% KM (Chebyshev) UCL	0.0899
k star	1.286	99% KM (Chebyshev) UCL	0.128
Theta star	0.019	Part of the table	
Nu star	15.44	Potential UCLs to Use	
AppChi2	7.567	95% KM (t) UCL	0.046
95% Gamma Approximate UCL (Use when n >= 40) 95% Adjusted Gamma UCL (Use when n < 40)	0.0498 N/A	95% KM (Percentile Bootstrap) UCL	0.0431

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Malchle, and Lee (2006).

For additional insight, the user may want to consult a statistician.

#### User Selected Options

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

#### SS\_Aluminum

#### General Statistics

Number of Valid Observations 6 Number of Distinct Observations 6

**Raw Statistics** Log-transformed Statistics Minimum of Log Data 7.601 Minimum 2000 Maximum 17000 Maximum of Log Data 9.741 Mean 5170 Mean of log Data 8.21 Geometric Mean 3678 SD of log Data 0.794 Median 2940 SD 5844 Std. Error of Mean 2386 Coefficient of Variation 1.13

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods! If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

95% Adjusted-CLT UCL (Chen-1995) 11551

95% Modified-t UCL (Johnson-1978) 10361

95% Adjusted Gamma UCL (Use when n < 40) 17716

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.611	Shapiro Wilk Test Statistic 0.78
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788
Data not Normal at 5% Significance Level	Data not Lognormal at 5% Significance Level
Assuming Normal Distribution	Assuming Lognormal Distribution
95% Student's-t UCL 9978	95% H-UCL 17226
95% UCLs (Adjusted for Skewness)	95% Chebyshev (MVLIF) LICL 11390

97.5% Chebyshev (MVUE) UCL 14267

99% Chebyshev (MVUE) UCL 19919

Gamma Distribution Test		Data Distribution
k star (bias corrected) 0		Data do not follow a Discernable Distribution (0.05)
Theta Star	5628	
MLE of Mean	5170	
MLE of Standard Deviation	5394	
nu star	11.02	
Approximate Chi Square Value (.05)	4.591	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 9094
Adjusted Chi Square Value	3.217	95% Jackknife UCL 9978
		95% Standard Bootstrap UCL 8796
Anderson-Darling Test Statistic	0.897	95% Bootstrap-t UCL 34096
Anderson-Darling 5% Critical Value	0.707	95% Hall's Bootstrap UCL 30866
Kolmogorov-Smirnov Test Statistic	0.358	95% Percentile Bootstrap UCL 9643
Kolmogorov-Smirnov 5% Critical Value	0.337	95% BCA Bootstrap UCL 10178
Data not Gamma Distributed at 5% Significance Le	vel	95% Chebyshev(Mean, Sd) UCL 15570
		97.5% Chebyshev(Mean, Sd) UCL 20069
Assuming Gamma Distribution		99% Chebyshev(Mean, Sd) UCL 28909
95% Approximate Gamma UCL (Use when n >= 40)	12414	

Potential UCL to Use Use 95% Chebyshev (Mean, Sd) UCL 15570

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL. These recommendations are based upon the results of the simulation studies summarized in Singh, Singh, and laci (2002) and Singh and Singh (2003). For additional insight, the user may want to consult a statistician.

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Anthracene

		General Statistics	
5	Number of Detected Data	6	Number of Valid Data
1	Number of Non-Detect Data	5	Number of Distinct Detected Data
16.67%	Percent Non-Detects		
	Log-transformed Statistics		Raw Statistics
-4.343	Minimum Detected	0.013	Minimum Detected
-2.733	Maximum Detected	0.065	Maximum Detected
-3.46	Mean of Detected	0.0386	Mean of Detected
0.753	SD of Detected	0.0248	SD of Detected
-2.631	Minimum Non-Detect	0.072	Minimum Non-Detect
-2.631	Maximum Non-Detect	0.072	Maximum Non-Detect

Warning: There are only 5 Detected Values in this data

Note: It should be noted that even though bootstrap may be performed on this data set
the resulting calculations may not be reliable enough to draw conclusions

It is recommended to have 10-15 or more distinct observations for accurate and meaningful results.

	UCL Statis	stics	
Normal Distribution Test with Detected Values Only		Lognormal Distribution Test with Detected Values On	ly
Shapiro Wilk Test Statistic	0.855	Shapiro Wilk Test Statistic	0.866
5% Shapiro Wilk Critical Value	0.762	5% Shapiro Wilk Critical Value	0.762
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level	
Assuming Normal Distribution		Assuming Lognormal Distribution	
DL/2 Substitution Method		DL/2 Substitution Method	
Mean	0.0382	Mean	-3.437
SD	0.0222	SD	0.675
95% DL/2 (t) UCL	0.0565	95% H-Stat (DL/2) UCL	0.103
Maximum Likelihood Estimate(MLE) Method	N/A	Log ROS Method	
MLE method falled to converge properly		Mean in Log Scale	-3.46
		SD in Log Scale	0.673
		Mean in Original Scale	0.0374
		SD in Original Scale	0.0224
		95% t UCL	0.0558
		95% Percentile Bootstrap UCL	0.0509
		95% BCA Bootstrap UCL	0.0512
		95% H-UCL	0.1
Gamma Distribution Test with Detected Values Only	y	Data Distribution Test with Detected Values Only	
k star (bias corrected)	1.168	Data appear Normal at 5% Significance Level	
Theta Star	0.033		
nu star	11.68		
A-D Test Statistic	0.435	Nonparametric Statistics	
5% A-D Critical Value	0.683	Kaplan-Meier (KM) Method	
K-S Test Statistic	0.683	Mean	0.0386
5% K-S Critical Value	0.36	SD	0.0222
Data appear Gamma Distributed at 5% Significance Lo	evel	SE of Mean	0.0111
		95% KM (t) UCL	0.061
Assuming Gamma Distribution		95% KM (z) UCL	0.0569
Gamma ROS Statistics using Extrapolated Data		95% KM (jackknife) UCL	0.0614
Minimum	0.013	95% KM (bootstrap t) UCL	0.0712
Maximum	0.065	95% KM (BCA) UCL	0.0548
Mean	0.0386	95% KM (Percentile Bootstrap) UCL	0.055
Median	0.0374	95% KM (Chebyshev) UCL	0.087
SD	0.0222	97.5% KM (Chebyshev) UCL	0.108
k star	1.649	99% KM (Chebyshev) UCL	0.149
Theta star	0.0234	B-s	
Nu star	19.79	Potential UCLs to Use	0.001
AppChi2	10.69	95% KM (t) UCL	0.061
95% Gamma Approximate UCL (Use when n >= 40)	0.0715	95% KM (Percentile Bootstrap) UCL	0.055
95% Adjusted Gamma UCL (Use when n < 40)	0.0911		
: DL/2 is not a recommended method.			

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).

For additional insight, the user may want to consult a statistician.

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Arsenic

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 5

#### Raw Statistics

Minimum 0.94
Maximum 5.7
Mean 2.24
Geometric Mean 1.858
Median 1.8
SD 1.747

SD 1.747 Std. Error of Mean 0.713 Coefficient of Variation 0.78 Skewness 2.126

#### Log-transformed Statistics

Minimum of Log Data -0.0619

Maximum of Log Data 1.74

Mean of log Data 0.62

SD of log Data 0.624

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.722 Shapiro Wilk Test Statistic 0.898
Shapiro Wilk Critical Value 0.788 Shapiro Wilk Critical Value 0.788
t 5% Significance Level Data appear Lognormal at 5% Significance Level

#### Data not Normal at 5% Significance Level

#### Assuming Normal Distribution Assuming Lognormal Distribution

95% Student's-t UCL 3.678
95% UCLs (Adjusted for Skewness)

 95% Adjusted-CLT UCL (Chen-1995) 4.075
 97.5% Chebyshev (MVUE) UCL 5.629

 95% Modified-t UCL (Johnson-1978) 3.781
 99% Chebyshev (MVUE) UCL 7.676

#### Gamma Distribution Test

## bution Test Data Distribution k star (bias corrected) 1.526 Data appear Gamma Distributed at 5% Significance Level Theta Star 1.468

MLE of Mean 2.24
MLE of Standard Deviation 1.813
nu star 18.32
Approximate Chi Square Value (.05) 9.619

Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 7.455

Anderson-Darling Test Statistic 0.545
Anderson-Darling 5% Critical Value 0.702
Kolmogorov-Smirnov Test Statistic 0.328
Kolmogorov-Smirnov 5% Critical Value 0.335
Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 4.265 95% Adjusted Gamma UCL (Use when n < 40) 5.503

#### Nonparametric Statistics

95% CLT UCL 3.413
95% Jackknife UCL 3.678
95% Standard Bootstrap UCL 3.313
95% Bootstrap-t UCL 6.082
95% Hall's Bootstrap UCL 8.67
95% Percentile Bootstrap UCL 3.54
95% BCA Bootstrap UCL 3.85
95% Chebyshev(Mean, Sd) UCL 5.35
97.5% Chebyshev(Mean, Sd) UCL 6.695

95% H-UCL 5.148

95% Chebyshev (MVUE) UCL 4.586

#### Potential UCL to Use

Use 95% Approximate Gamma UCL 4.265

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Singh, and laci (2002) and Singh and Singh (2003). For additional insight, the user may want to consult a statistician.

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Barlum

Data

95% Adjusted Gamma UCL (Use when n < 40) 975.4

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

Raw Statistics		Log-transformed Statistics
Minimum	81.4	Minimum of Log Data 4.399
Maximum	809	Maximum of Log Data 6.696
Mean	310.4	Mean of log Data 5.442
Geometric Mean	230.9	SD of log Data 0.844
Median	249.5	
SD	268.8	
Std. Error of Mean	109.7	
Coefficient of Variation	0.866	
Skewness	1.573	

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

		•
	Relevant UCL	Statistics
Normal Distribution Test		Lognormal Distribution Test
Shapiro Wilk Test Statistic	0.839	Shapiro Wilk Test Statistic 0.967
Shapiro Wilk Critical Value	0.788	Shapiro Wilk Critical Value 0.788
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level
Assuming Normal Distribution		Assuming Lognormal Distribution
95% Student's-t UCL	531.5	95% H-UCL 1288
95% UCLs (Adjusted for Skewness)		95% Chebyshev (MVUE) UCL 764.3
95% Adjusted-CLT UCL (Chen-1995)	566.2	97.5% Chebyshev (MVUE) UCL 962.1
95% Modified-t UCL (Johnson-1978)	543.3	99% Chebyshev (MVUE) UCL 1351
Gamma Distribution Test		Data Distribution
k star (bias corrected)	1.03	Data appear Normal at 5% Significance Level
Theta Star	301.2	
MLE of Mean	310.4	
MLE of Standard Deviation	305.8	
nu star	12.37	
Approximate Chi Square Value (.05)	5.469	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 490.9
Adjusted Chi Square Value	3.935	95% Jackknife UCL 531.5
		95% Standard Bootstrap UCL 473.6
Anderson-Darling Test Statistic	0.264	95% Bootstrap-t UCL 728.9
Anderson-Darling 5% Critical Value	0.705	95% Hall's Bootstrap UCL 1165
Kolmogorov-Smirnov Test Statistic	0.177	95% Percentile Bootstrap UCL 492.2
Kolmogorov-Smirnov 5% Critical Value	0.336	95% BCA Bootstrap UCL 537.5
a appear Gamma Distributed at 5% Significance	Level	95% Chebyshev(Mean, Sd) UCL 788.7
		97.5% Chebyshev(Mean, Sd) UCL 995.7
Assuming Gamma Distribution		99% Chebyshev(Mean, Sd) UCL 1402
5% Approximate Gamma UCL (Use when n >= 40)	701.9	

Potential UCL to Use Use 95% Student's-t UCL 531.5

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Singh, and Iacl (2002) and Singh and Singh (2003). For additional insight, the user may want to consult a statistician.

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Benzo(a)anthracene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 5

Raw	Ctal	اهماه	

 Minimum
 0.063
 Minimum of Log Data -2.765

 Maximum
 0.59
 Maximum of Log Data -0.528

 Mean
 0.237
 Mean of log Data -1.854

 Geometric Mean
 0.157
 SD of log Data 0.972

 Median
 0.1
 SD 0.237

 Std. Error of Mean
 0.0967

SD 0.237 Std. Error of Mean 0.0967 Coefficient of Variation 0.998 Skewness 1.03

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.733	Shapiro Wilk Test Statistic 0.799
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788
Data not Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level
Assuming Normal Distribution	Assuming Lognormal Distribution
95% Student's-t UCL 0.432	95% H-UCL 1.444
95% UCLs (Adjusted for Skewness)	95% Chebyshev (MVUE) UCL 0.616
95% Adjusted-CLT UCL (Chen-1995) 0.44	97.5% Chebyshev (MVUE) UCL 0.783
95% Modified-t UCL (Johnson-1978) 0.439	99% Chebyshev (MVUE) UCL 1.113

#### Gamma Distribution Test Data Distribution

Gamma Distribution Test		Data Distribution
k star (bias corrected)	0.784	Data appear Lognormal at 5% Significance Level
Theta Star	0.303	
MLE of Mean	0.237	
MLE of Standard Deviation	0.268	
nu star	9.403	
Approximate Chi Square Value (.05)	3.572	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 0.396

Adjusted Chi Square Value 2.403	95% Jackknife UCL 0.432
	95% Standard Bootstrap UCL 0.382
Anderson-Darling Test Statistic 0.809	95% Bootstrap-t UCL 2.474
Anderson-Darling 5% Critical Value 0.71	95% Hall's Bootstrap UCL 2.875
Kolmogorov-Smirnov Test Statistic 0.383	95% Percentile Bootstrap UCL 0.39
Kolmogorov-Smirnov 5% Critical Value 0.339	95% BCA Bootstrap UCL 0.407
Data not Gamma Distributed at 5% Significance Level	95% Chebyshev(Mean, Sd) UCL 0.659
	97.5% Chebyshev(Mean, Sd) UCL 0.841

### Assuming Gamma Distribution 95% Approximate Gamma UCL (Use when n >= 40) 0.625

95% Adjusted Gamma UCL (Use when n < 40) 0.929

Use 95% H-UCL 1.444

99% Chebyshev(Mean, Sd) UCL 1.2

#### Potential UCL to Use

Recommended UCL exceeds the maximum observation

ProUCL computes and outputs H-statistic based UCLs for historical reasons only.

H-statistic often results in unstable (both high and low) values of UCL95 as shown in examples in the Technical Guide.

It is therefore recommended to avoid the use of H-statistic based 95% UCLs.

Use of nonparametric methods are preferred to compute UCL95 for skewed data sets which do not follow a gamma distribution.

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Singh, and laci (2002) and Singh and Singh (2003). For additional insight, the user may want to consult a statistician.

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Benzo(a)pyrene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics**

Minimum 0.053 Maximum 0.5 Mean 0.224 Geometric Mean 0.158 Median 0.13 SD 0.198

SD 0.198 Std. Error of Mean 0.0809 Coefficient of Variation 0.885 Skewness 0.867

#### Log-transformed Statistics

Minimum of Log Data -2.937 Maximum of Log Data -0.693 Mean of log Data -1.846 SD of log Data 0.924

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

### Relevant UCL Statistics

Normal	Distribution	Test

Shapiro Wilk Test Statistic 0.799 Shapiro Wilk Critical Value 0.788

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Shapiro Wilk Test Statistic 0.904 Shapiro Wilk Critical Value 0.788

#### Data appear Lognormal at 5% Significance Level

Lognormal Distribution Test

# Data appear Normal at 5% Significance Level Assuming Normal Distribution

95% Student's-t UCL 0.387

# 95% UCLs (Adjusted for Skewness)

95% Adjusted-CLT UCL (Chen-1995) 0.388 95% Modified-t UCL (Johnson-1978) 0.392

# Assuming Lognormal Distribution

95% H-UCL 1.185 95% Chebyshev (MVUE) UCL 0.581 97.5% Chebyshev (MVUE) UCL 0.737 99% Chebyshev (MVUE) UCL 1.042

#### Gamma Distribution Test

k star (bias corrected) 0.899 Theta Star 0.249

MLE of Mean 0.224
MLE of Standard Deviation 0.236

nu star 10.79 Approximate Chi Square Value (.05) 4.439

> Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 3.094

Anderson-Darling Test Statistic 0.473
Anderson-Darling 5% Critical Value 0.707
Kolmogorov-Smirnov Test Statistic 0.233
Kolmogorov-Smirnov 5% Critical Value 0.337
Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 0.544 95% Adjusted Gamma UCL (Use when n < 40) 0.781

#### Data Distribution

Data appear Normal at 5% Significance Level

#### Nonparametric Statistics

95% Jackknife UCL 0.387
95% Standard Bootstrap UCL 0.346
95% Bootstrap-t UCL 0.804
95% Hall's Bootstrap UCL 1.441
95% Percentile Bootstrap UCL 0.352
95% BCA Bootstrap UCL 0.361
95% Chebyshev(Mean, Sd) UCL 0.577
97.5% Chebyshev(Mean, Sd) UCL 0.729
99% Chebyshev(Mean, Sd) UCL 1.029

95% CLT UCL 0.357

#### Potential UCL to Use

Use 95% Student's-t UCL 0.387

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

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#### SS\_Benzo(b)fluoranthene

#### General Statistics

Number of Valid Observations 6 Number of Distinct Observations 6

aw Statistics	Log-transformed Statisti
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 Minimum
 0.1
 Minimum of Log Data
 -2.303

 Maximum
 0.82
 Maximum of Log Data
 -0.198

 Mean
 0.39
 Mean of log Data
 -1.255

 Geometric Mean
 0.285
 SD of log Data
 0.871

 Median
 0.235

 SD
 0.33

 Std. Error of Mean
 0.135

 Coefficient of Variation
 0.846

 Skewness
 0.854

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.776	Shapiro Wilk Test Statistic 0.894
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788

Data not Normal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

### Assuming Normal Distribution Assuming Lognormal Distribution

 95% Student's-t UCL 0.661
 95% H-UCL 1.751

 95% UCLs (Adjusted for Skewness)
 95% Chebyshev (MVUE) UCL 0.978

 95% Adjusted-CLT UCL (Chen-1995) 0.662
 97.5% Chebyshev (MVUE) UCL 1.234

 95% Modified-t UCL (Johnson-1978) 0.669
 99% Chebyshev (MVUE) UCL 1.738

#### Gamma Distribution Test Data Distribution

k star (bias corrected) 0.983 Data appear Gamma Distributed at 5% Significance Level

Theta Star 0.397

MLE of Mean 0.39
MLE of Standard Deviation 0.393

nu star 11.8

Approximate Chi Square Value (.05) 5.095 Nonparametric Statistics

Adjusted Level of Significance 0.0122 95% CLT UCL 0.611

Adjusted Chi Square Value 3.628 95% Jackknife UCL 0.661 95% Standard Bootstrap UCL 0.596 Anderson-Darling Test Statistic 0.514 95% Bootstrap+t UCL 1.489

Anderson-Darling 5% Critical Value 0.706 95% Hall's Bootstrap UCL 2.953
Kolmogorov-Smirnov Test Statistic 0.261 95% Percentile Bootstrap UCL 0.603
Kolmogorov-Smirnov 5% Critical Value 0.337 95% BCA Bootstrap UCL 0.612

Data appear Gamma Distributed at 5% Significance Level 95% Chebyshev(Mean, Sd) UCL 0.977

97.5% Chebyshev(Mean, Sd) UCL 1.231

Assuming Gamma Distribution 99% Chebyshev(Mean, Sd) UCL 1.73

# 95% Approximate Gamma UCL (Use when n >= 40) 0.903

95% Adjusted Gamma UCL (Use when n < 40) 1.268

Use 95% Approximate Gamma UCL 0.903

Potential UCL to Use

Use

Recommended UCL exceeds the maximum observation

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Benzo(g,h,i)perylene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 5

#### **Raw Statistics**

Minimum 0.022
Maximum 0.21
Mean 0.115
Geometric Mean 0.083
Median 0.108
SD 0.0859
Std. Error of Mean 0.0351

Coefficient of Variation 0.745

Log-transformed Statistics

Minimum of Log Data -3.817

Maximum of Log Data -1.561

Mean of log Data -2.489

SD of log Data 0.968

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test	
Shapiro Wilk Test Statistic 0.855	Shapiro Wilk Test Statistic 0.883	
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788	
Data appear Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level	

#### Assuming Normal Distribution

95% Student's-t UCL 0.186

95% UCLs (Adjusted for Skewness)

95% Adjusted-CLT UCL (Chen-1995) 0.175

95% Modified-t UCL (Johnson-1978) 0.186

# Assuming Lognormal Distribution

95% H-UCL 0.751 95% Chebyshev (MVUE) UCL 0.324 97.5% Chebyshev (MVUE) UCL 0.413 99% Chebyshev (MVUE) UCL 0.586

#### Gamma Distribution Test

Theta Star 0.122
MLE of Mean 0.115
MLE of Standard Deviation 0.119
nu star 11.33
Approximate Chi Square Value (.05) 4.789

Adjusted Level of Significance 0.0122

Anderson-Darling Test Statistic 0.419

Adjusted Chi Square Value 3.378

k star (bias corrected) 0.944

# Data Distribution Data appear Normal at 5% Significance Level

| 95% CLT UCL | 0.173 | 95% CLT UCL | 0.186 | 95% Standard Bootstrap UCL | 0.186 | 95% Standard Bootstrap UCL | 0.168 | 95% Bootstrap-t UCL | 0.162 | 95% Hall's Bootstrap UCL | 0.164 | 95% Percentile Bootstrap UCL | 0.166 | 95% Chebyshev(Mean, Sd) UCL | 0.268 |

97.5% Chebyshev(Mean, Sd) UCL 0.334 99% Chebyshev(Mean, Sd) UCL 0.464

Anderson-Darling 5% Critical Value 0.707
Kolmogorov-Smirnov Test Statistic 0.229
Kolmogorov-Smirnov 5% Critical Value 0.337

Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 0.273 95% Adjusted Gamma UCL (Use when n < 40) 0.387

Use 95% Student's-t UCL 0.186

#### Potential UCL to Use

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Benzo(k)fluoranthene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics**

Minimum 0.028
Maximum 0.27
Mean 0.115
Geometric Mean 0.081
Median 0.0635
SD 0.103
Std. Error of Mean 0.0421

Coefficient of Variation 0.9

Log-transformed Statistics

Minimum of Log Data -3.576 Maximum of Log Data -1.309 Mean of log Data -2.513 SD of log Data 0.91

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test	
Shapiro Wilk Test Statistic 0.803	Shapiro Wilk Test Statistic 0.908	
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788	
Data appear Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level	

#### Assuming Normal Distribution

95% Student's-t UCL 0.2

95% UCLs (Adjusted for Skewness)

95% Adjusted-CLT UCL (Chen-1995) 0.202

95% Modified-t UCL (Johnson-1978) 0.202

#### Assuming Lognormal Distribution

95% H-UCL 0.576 95% Chebyshev (MVUE) UCL 0.293 97.5% Chebyshev (MVUE) UCL 0.371 99% Chebyshev (MVUE) UCL 0.524

#### Gamma Distribution Test

Theta Star 0.127
MLE of Mean 0.115
MLE of Standard Deviation 0.121
nu star 10.85
Approximate Chi Square Value (.05) 4.481

Adjusted Level of Significance 0.0122

Adjusted Chi Square Value 3.128

k star (bias corrected) 0.904

# Data appear Normal at 5% Significance Level

**Data Distribution** 

95% CLT UCL 0.184
95% Jackknife UCL 0.2
95% Standard Bootstrap UCL 0.178
95% Bootstrap-t UCL 0.525
95% Hall's Bootstrap UCL 0.825
95% Percentile Bootstrap UCL 0.188
95% BCA Bootstrap UCL 0.188
95% Chebyshev(Mean, Sd) UCL 0.298
97.5% Chebyshev(Mean, Sd) UCL 0.378

99% Chebyshev(Mean, Sd) UCL 0.534

Anderson-Darling Test Statistic 0.482
Anderson-Darling 5% Critical Value 0.707
Kolmogorov-Smirnov Test Statistic 0.272
Kolmogorov-Smirnov 5% Critical Value 0.337

Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 0.278 95% Adjusted Gamma UCL (Use when n < 40) 0.398

Use 95% Student's-t UCL 0.2

Potential UCL to Use

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

SS\_Calcium

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics**

Minimum 21700 Maximum 264000 Mean 134767 Geometric Mean 100189 Median 133850 SD 93857

Std. Error of Mean 38317 Coefficient of Variation 0.696

#### Log-transformed Statistics

Minimum of Log Data 9.985 Maximum of Log Data 12.48 Mean of log Data 11.51 SD of log Data 0.943

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methods! If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal	Distribution	Test
HOIIIIGI	Diautibution	100

Shapiro Wilk Test Statistic 0.945 Shapiro Wilk Critical Value 0.788

# Data appear Normal at 5% Significance Level

**Assuming Normal Distribution** 95% Student's-t UCL 211977

95% UCLs (Adjusted for Skewness)

95% Adjusted-CLT UCL (Chen-1995) 200711 95% Modified-t UCL (Johnson-1978) 212432

# Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.922 Shapiro Wilk Critical Value 0.788 Data appear Lognormal at 5% Significance Level

#### Assuming Lognormal Distribution

95% H-UCL 814145 95% Chebyshev (MVUE) UCL 378499 97.5% Chebyshev (MVUE) UCL 480588 99% Chebyshev (MVUE) UCL 681124

#### Gamma Distribution Test

k star (bias corrected) 1.029 Theta Star 130985

MLE of Mean 134767 MLE of Standard Deviation 132862 nu star 12.35

Approximate Chi Square Value (.05) 5.456 Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 3.924

Anderson-Darling Test Statistic 0.276 Anderson-Darling 5% Critical Value 0.705 Kolmogorov-Smirnov Test Statistic 0.244 Kolmogorov-Smirnov 5% Critical Value 0.336 Data appear Gamma Distributed at 5% Significance Level

#### **Assuming Gamma Distribution**

95% Approximate Gamma UCL (Use when n >= 40) 304961 95% Adjusted Gamma UCL (Use when n < 40) 423978

**Data Distribution** Data appear Normal at 5% Significance Level

#### Nonparametric Statistics

95% CLT UCL 197792 95% Jackknife UCL 211977 95% Standard Bootstrap UCL 192861 95% Bootstrap-t UCL 221742 95% Hall's Bootstrap UCL 185111 95% Percentile Bootstrap UCL 193700 95% BCA Bootstrap UCL 193700 95% Chebyshev(Mean, Sd) UCL 301786 97.5% Chebyshev(Mean, Sd) UCL 374055 99% Chebyshev(Mean, Sd) UCL 516014

#### Potential UCL to Use

Use 95% Student's-t UCL 211977

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

#### SS Chromium

#### **General Statistics**

Number of Valid Observations 6 Number of Distinct Observations 6

**Raw Statistics** Log-transformed Statistics

Minimum 2 Minimum of Log Data 0.693 Maximum 17.6 Maximum of Log Data 2.868 Mean 8.083 Mean of log Data 1.779 Geometric Mean 5.923 SD of log Data 0.863 Median 4.35 SD 6.899 Std. Error of Mean 2.817 Coefficient of Variation 0.854

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

Skewness 0.913

It is suggested to collect at least 8 to 10 observations using these statistical methodsl If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Normal Distribution Test	Lognormai Distribution Test

Shapiro Wilk Test Statistic 0.762 Shapiro Wilk Test Statistic 0.864 Shapiro Wilk Critical Value 0.788 Shapiro Wilk Critical Value 0.788

Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

Assuming Normal Distribution Assuming Lognormal Distribution

95% Student's-t UCL 13.76 95% H-UCL 35.3 95% UCLs (Adjusted for Skewness) 95% Chebyshev (MVUE) UCL 20.1 95% Adjusted-CLT UCL (Chen-1995) 13.84 97.5% Chebyshev (MVUE) UCL 25.34 95% Modified-t UCL (Johnson-1978) 13.93 99% Chebyshev (MVUE) UCL 35.65

Gamma Distribution Test **Data Distribution** 

k star (bias corrected) 0.989 Data Follow Appr. Gamma Distribution at 5% Significance Level Theta Star 8.173

MLF of Mean 8 083

MLE of Standard Deviation 8.128

nu star 11.87

Approximate Chi Square Value (.05) 5.14 Nonparametric Statistics

95% CLT UCL 12.72 Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 3.665 95% Jackknife UCL 13.76

95% Standard Bootstrap UCL 12.33 Anderson-Darling Test Statistic 0.653 95% Bootstrap-t UCL 38.14 Anderson-Darling 5% Critical Value 0.706 95% Hall's Bootstrap UCL 79.37

99% Chebyshev(Mean, Sd) UCL 36.11

Kolmogorov-Smirnov Test Statistic 0.347 95% Percentile Bootstrap UCL 12.55 Kolmogorov-Smirnov 5% Critical Value 0.337 95% BCA Bootstrap UCL 12.72 Data follow Appr. Gamma Distribution at 5% Significance Level 95% Chebyshev(Mean, Sd) UCL 20.36 97.5% Chebyshev(Mean, Sd) UCL 25.67

Assuming Gamma Distribution 95% Approximate Gamma UCL (Use when n >= 40) 18.66 95% Adjusted Gamma UCL (Use when n < 40) 26.18

> Potential UCL to Use Use 95% Approximate Gamma UCL 18.66

Recommended UCL exceeds the maximum observation

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Chrysene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics**

Minimum 0.07
Maximum 0.6
Mean 0.267
Geometric Mean 0.192
Median 0.155
SD 0.232
Std. Error of Mean 0.0947

Coefficient of Variation 0.87

Log-transformed Statistics

Minimum of Log Data -2.659

Maximum of Log Data -0.511

Mean of log Data -1.651

SD of log Data 0.889

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test	
Shapiro Wilk Test Statistic 0.803	Shapiro Wilk Test Statistic 0.898	
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788	
Data appear Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level	

#### Assuming Normal Distribution

95% Student's-t UCL 0.458

95% UCLs (Adjusted for Skewness)

95% Adjusted-CLT UCL (Chen-1995) 0.46

95% Modified-t UCL (Johnson-1978) 0.463

#### Assuming Lognormal Distribution

95% H-UCL 1.26 95% Chebyshev (MVUE) UCL 0.674 97.5% Chebyshev (MVUE) UCL 0.853 99% Chebyshev (MVUE) UCL 1.202

#### Gamma Distribution Test

Theta Star 0.283

MLE of Mean 0.267

MLE of Standard Deviation 0.275

nu star 11.32

Approximate Chi Square Value (.05) 4.783

Adjusted Level of Significance 0.0122

Adjusted Chi Square Value 3.373

k star (bias corrected) 0.943

**Data Distribution** 

Data appear Normal at 5% Significance Level

95% CLT UCL 0.422
95% Jackknife UCL 0.458
95% Standard Bootstrap UCL 0.409
95% Bootstrap-t UCL 1.011
95% Hall's Bootstrap UCL 1.581
95% Percentile Bootstrap UCL 0.418
95% BCA Bootstrap UCL 0.43
95% Chebyshev(Mean, Sd) UCL 0.68
97.5% Chebyshev(Mean, Sd) UCL 0.858

# Anderson-Darling Test Statistic 0.485 Anderson-Darling 5% Critical Value 0.707 Kolmogorov-Smirnov Test Statistic 0.237 Kolmogorov-Smirnov 5% Critical Value 0.337

Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 0.631 95% Adjusted Gamma UCL (Use when n < 40) 0.895

Potential UCL to Use

Use 95% Student's-t UCL 0.458

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

SS\_Cobalt

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics**

Minimum 0.72
Maximum 3.8
Mean 1.577
Geometric Mean 1.32
Median 1.195
SD 1.157
Std. Error of Mean 0.473

Coefficient of Variation 0.734

Log-transformed Statistics

Minimum of Log Data -0.329

Maximum of Log Data 1.335

Mean of log Data 0.277

SD of log Data 0.619

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

### Relevant UCL Statistics

Data not Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level	
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788	
Shapiro Wilk Test Statistic 0.771	Shapiro Wilk Test Statistic 0.896	
Normal Distribution Test	Lognormal Distribution Test	

#### Assuming Normal Distribution

95% UCLs (Adjusted for Skewness) 95% Adjusted-CLT UCL (Chen-1995) 2.739 95% Modified-t UCL (Johnson-1978) 2.589

95% Student's-t UCL 2.529

95% H-UCL 3.608 95% Chebyshev (MVUE) UCL 3.236 97.5% Chebyshev (MVUE) UCL 3.969 99% Chebyshev (MVUE) UCL 5.408

# Gamma Distribution Test

k star (bias corrected) 1.593
Theta Star 0.99
MLE of Mean 1.577
MLE of Standard Deviation 1.249
nu star 19.12

Data Distribution

Data appear Gamma Distributed at 5% Significance Level

Assuming Lognormal Distribution

# Approximate Chi Square Value (.05) 10.2 Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 7.963

Anderson-Darling Test Statistic 0.475
Anderson-Darling 5% Critical Value 0.701
Kolmogorov-Smirnov Test Statistic 0.257
Kolmogorov-Smirnov 5% Critical Value 0.335
Data appear Gamma Distributed at 5% Significance Level

## Nonparametric Statistics

95% CLT UCL 2.354
95% Jackknife UCL 2.529
95% Standard Bootstrap UCL 2.272
95% Bootstrap-t UCL 3.523
95% Hall's Bootstrap UCL 5.165
95% Percentile Bootstrap UCL 2.367
95% BCA Bootstrap UCL 2.582
95% Chebyshev(Mean, Sd) UCL 3.636
97.5% Chebyshev(Mean, Sd) UCL 4.527
99% Chebyshev(Mean, Sd) UCL 6.278

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 2.954 95% Adjusted Gamma UCL (Use when n < 40) 3.786

Potential UCL to Use

Use 95% Approximate Gamma UCL 2.954

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Copper

#### General Statistics

Number of Valid Observations 6 Number of Distinct Observations 6

Raw Statistics

 Minimum
 2.8
 Minimum of Log Data
 1.03

 Maximum
 39.8
 Maximum of Log Data
 3.684

 Mean
 16.07
 Mean of log Data
 2.224

 Geometric Mean
 9.246
 SD of log Data
 1.14

 Median
 5.45
 5.45
 5.45

Log-transformed Statistics

Median 5.45 SD 17.69 Std. Error of Mean 7.221 Coefficient of Variation 1.101 Skewness 0.959

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Tes

Shapiro Wilk Test Statistic 0.7 Shapiro Wilk Test Statistic 0.805
Shapiro Wilk Critical Value 0.788 Shapiro Wilk Critical Value 0.788

Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

Assuming Normal Distribution Assuming Lognormal Distribution

 95% Student's-t UCL 30.62
 95% H-UCL 186.2

 95% UCLs (Adjusted for Skewness)
 95% Chebyshev (MVUE) UCL 45.61

 95% Adjusted-CLT UCL (Chen-1995) 30.96
 97.5% Chebyshev (MVUE) UCL 58.72

 95% Modified-t UCL (Johnson-1978) 31.09
 99% Chebyshev (MVUE) UCL 84.46

Gamma Distribution Test Data Distribution

k star (bias corrected) 0.631 Data appear Lognormal at 5% Significance Level
Theta Star 25.46

MI F of Mean 16.07

MLE of Standard Deviation 20.23

95% Adjusted Gamma UCL (Use when n < 40) 77.55

nu star 7.572

Approximate Chi Square Value (.05) 2.49 Nonparametric Statistics

Adjusted Level of Significance 0.0122 95% CLT UCL 27.94
Adjusted Chi Square Value 1.569 95% Jackknife UCL 30.62

Anderson-Darling Test Statistic 0.836
Anderson-Darling 5% Critical Value 0.715
Kolmogorov-Smirnov Test Statistic 0.372

Kolmogorov-Smirnov 5% Critical Value 0.341

95% Standard Bootstrap UCL 26.75
95% Bootstrap-t UCL 184
95% Hall's Bootstrap UCL 263.2
95% Percentile Bootstrap UCL 27.58

Data not Gamma Distributed at 5% Significance Level 95% Chebyshev (Mean, Sd.) UCL 47.54

97.5% Chebyshev(Mean, Sd) UCL 61.16

Assuming Gamma Distribution 99% Chebyshev (Mean, Sd) UCL 87.91 95% Approximate Gamma UCL (Use when n >= 40) 48.86

Potential UCL to Use Use 95% Chebyshev (Mean, Sd) UCL 47.54

Recommended UCL exceeds the maximum observation

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Dibenz(a,h)anthracene

	General Sta	ntistics	
Number of Valid Data	6	Number of Detected Data	5
Number of Distinct Detected Data	5	Number of Non-Detect Data	1
		Percent Non-Detects	16.67%
Raw Statistics		Log-transformed Statistics	
Minimum Detected	0.01	Minimum Detected	-4.605
Maximum Detected	0.076	Maximum Detected	-2.577
Mean of Detected	0.0472	Mean of Detected	-3.305
SD of Detected	0.0302	SD of Detected	0.884
Minimum Non-Detect	0.072	Minimum Non-Detect	-2.631
Maximum Non-Detect	0.072	Maximum Non-Detect	-2.631

Warning: There are only 5 Detected Values in this data

Note: It should be noted that even though bootstrap may be performed on this data set
the resulting calculations may not be reliable enough to draw conclusions

It is recommended to have 10-15 or more distinct observations for accurate and meaningful results.

	UCL Statist	nice.	
Normal Distribution Test with Detected Values Only		Lognormal Distribution Test with Detected Values Onl	v
Shapiro Wilk Test Statistic	0.878	Shapiro Wilk Test Statistic	0.864
5% Shapiro Wilk Critical Value	0.762	5% Shapiro Wilk Critical Value	0.762
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level	
Assuming Normal Distribution		Assuming Lognormal Distribution	
DL/2 Substitution Method		DL/2 Substitution Method	
Mean	0.0453	Mean	-3.308
SD	0.0274	SD	0.791
95% DL/2 (t) UCL	0.0679	95% H-Stat (DL/2) UCL	0.169
Maximum Likelihood Estimate(MLE) Method	N/A	Log ROS Method	
MLE method falled to converge properly		Mean in Log Scale	-3.39
		SD in Log Scale	0.818
		Mean in Original Scale	0.043
		SD in Original Scale	0.0289
		95% t UCL	0.0668
		95% Percentile Bootstrap UCL	0.0608
		95% BCA Bootstrap UCL	0.0608
		95% H-UCL	0.171
Gamma Distribution Test with Detected Values Only	y	Data Distribution Test with Detected Values Only	
k star (bias corrected)	0.988	Data appear Normal at 5% Significance Level	
Theta Star	0.0478		
nu star	9.878		
A-D Test Statistic	0.421	Nonparametric Statistics	
5% A-D Critical Value	0.684	Kaplan-Meier (KM) Method	
K-S Test Statistic	0.684	Mean	0.0441
5% K-S Critical Value	0.36	SD	0.0267
Data appear Gamma Distributed at 5% Significance Lo	evel	SE of Mean	0.0128
		95% KM (t) UCL	0.0698
Assuming Gamma Distribution		95% KM (z) UCL	0.0651
Gamma ROS Statistics using Extrapolated Data		95% KM (jackknife) UCL	0.0705
		95% KM (bootstrap t) UCL	0.068
Minimum	0.01	95 % KW (bootstrap t) OCL	0.000
Minimum Maximum	0.01	95% KM (BCA) UCL	0.0643
Maximum	0.076	95% KM (BCA) UCL	0.0643
Maximum Mean	0.076 0.0439 0.0402 0.0282	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL	0.0643 0.0643
Maximum Mean Median SD k star	0.076 0.0439 0.0402 0.0282 1.283	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL 95% KM (Chebyshev) UCL	0.0643 0.0643 0.0998
Maximum Mean Median SD	0.076 0.0439 0.0402 0.0282 1.283 0.0342	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL 95% KM (Chebyshev) UCL 97.5% KM (Chebyshev) UCL 99% KM (Chebyshev) UCL	0.0643 0.0643 0.0998 0.124
Maximum Mean Median SD k star	0.076 0.0439 0.0402 0.0282 1.283	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL 95% KM (Chebyshev) UCL 97.5% KM (Chebyshev) UCL	0.0643 0.0643 0.0998 0.124
Maximum Mean Median SD k star Theta star	0.076 0.0439 0.0402 0.0282 1.283 0.0342	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL 95% KM (Chebyshev) UCL 97.5% KM (Chebyshev) UCL 99% KM (Chebyshev) UCL	0.0643 0.0643 0.0998 0.124
Maximum Mean Median SD k star Theta star Nu star AppChi2 95% Gamma Approximate UCL (Use when n >= 40)	0.076 0.0439 0.0402 0.0282 1.283 0.0342 15.39 7.534 0.0896	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL 95% KM (Chebyshev) UCL 97.5% KM (Chebyshev) UCL 99% KM (Chebyshev) UCL	0.0643 0.0643 0.0998 0.124 0.171
Maximum Mean Median SD k star Theta star Nu star AppChi2	0.076 0.0439 0.0402 0.0282 1.283 0.0342 15.39 7.534	95% KM (BCA) UCL 95% KM (Percentile Bootstrap) UCL 95% KM (Chebyshev) UCL 97.5% KM (Chebyshev) UCL 99% KM (Chebyshev) UCL Potential UCLs to Use 95% KM (t) UCL	0.0643 0.0643 0.0998 0.124 0.171

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Fluoranthene

#### General Statistics

Number of Valid Observations 6

Number of Distinct Observations 6

Log-transformed Statistics

w	Statistics		

 Minimum 0.16
 Minimum of Log Data -1.833

 Maximum 1.4
 Maximum of Log Data 0.336

 Mean 0.525
 Mean of log Data -1.035

 Geometric Mean 0.355
 SD of log Data 0.932

 Median 0.23
 SD 0.524

 Std. Error of Mean 0.214
 Std. Error of Variation 0.998

 Skewness 1.261
 Skewness 1.261

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set,

the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistic

Relevant UCL Statistics		
Normal Distribution Test		Lognormal Distribution Test
Shapiro Wilk Test Statistic	0.753	Shapiro Wilk Test Statistic 0.811
Shapiro Wilk Critical Value	0.788	Shapiro Wilk Critical Value 0.788
Data not Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level
Assuming Normal Distribution		Assuming Lognormal Distribution
95% Student's-t UCL	0.956	95% H-UCL 2.764
95% UCLs (Adjusted for Skewness)		95% Chebyshev (MVUE) UCL 1.323
95% Adjusted-CLT UCL (Chen-1995)	0.995	97.5% Chebyshev (MVUE) UCL 1.679
95% Modified-t UCL (Johnson-1978)	0.974	99% Chebyshev (MVUE) UCL 2.377
Gamma Distribution Test		Data Distribution
k star (bias corrected)	0.823	Data appear Lognormal at 5% Significance Level
Theta Star	0.638	
MLE of Mean	0.525	
MLE of Standard Deviation	0.579	
nu star	9.878	
Approximate Chi Square Value (.05)	3.866	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 0.877
Adjusted Chi Square Value	2.635	95% Jackknife UCL 0.956
		95% Standard Bootstrap UCL 0.846
Anderson-Darling Test Statistic	0.736	95% Bootstrap-t UCL 5.363
Anderson-Darling 5% Critical Value	0.709	95% Hall's Bootstrap UCL 4.433
Kolmogorov-Smirnov Test Statistic	0.356	95% Percentile Bootstrap UCL 0.855
Kolmogorov-Smirnov 5% Critical Value	0.338	95% BCA Bootstrap UCL 0.927
a not Gamma Distributed at 5% Significance Le	evel	95% Chebyshev(Mean, Sd) UCL 1.458
		97.5% Chebyshev(Mean, Sd) UCL 1.861

#### Potential UCL to Use

Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 1.342 95% Adjusted Gamma UCL (Use when n < 40) 1.968

Use 95% H-UCL 2.764

99% Chebyshev(Mean, Sd) UCL 2.654

Recommended UCL exceeds the maximum observation

ProUCL computes and outputs H-statistic based UCLs for historical reasons only.

H-statistic often results in unstable (both high and low) values of UCL95 as shown in examples in the Technical Guide.

It is therefore recommended to avoid the use of H-statistic based 95% UCLs.

Use of nonparametric methods are preferred to compute UCL95 for skewed data sets which do not follow a gamma distribution.

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Indeno(1,2,3-cd)pyrene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 5

#### **Raw Statistics**

Minimum 0.05 Maximum 0.35 Mean 0.18 Geometric Mean 0.139 Median 0.13

SD 0.136 Std. Error of Mean 0.0556 Coefficient of Variation 0.756 Skewness 0.706

#### Log-transformed Statistics

Minimum of Log Data -2.996

Maximum of Log Data -1.05

Mean of log Data -1.977

SD of log Data 0.81

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal	Distribution	Test

Assuming Normal Distribution

Shapiro Wilk Test Statistic 0.817 Shapiro Wilk Critical Value 0.788

# Data appear Normal at 5% Significance Level

95% Student's-t UCL 0.292

95% UCLs (Adjusted for Skewness)
95% Adjusted-CLT UCL (Chen-1995) 0.288
95% Modified-t UCL (Johnson-1978) 0.295

# Gamma Distribution Test

Theta Star 0.158

MLE of Mean 0.18

MLE of Standard Deviation 0.168

k star (bias corrected) 1.142

nu star 13.7

Approximate Chi Square Value (.05) 6.369

Adjusted Level of Significance 0.0122

Adjusted Chi Square Value 4.683

Anderson-Darling Test Statistic 0.403

Anderson-Darling 5% Critical Value 0.704

Kolmogorov-Smirnov Test Statistic 0.235

Kolmogorov-Smirnov 5% Critical Value 0.336

Data appear Gamma Distributed at 5% Significance Level

# Assuming Gamma Distribution

Potential UCL to Use

95% Approximate Gamma UCL (Use when n >= 40) 0.387 95% Adjusted Gamma UCL (Use when n < 40) 0.527

#### Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.912 Shapiro Wilk Critical Value 0.788

#### Data appear Lognormal at 5% Significance Level

# Assuming Lognormal Distribution

95% H-UCL 0.686 95% Chebyshev (MVUE) UCL 0.438 97.5% Chebyshev (MVUE) UCL 0.55 99% Chebyshev (MVUE) UCL 0.769

#### Data Distribution

Data appear Normal at 5% Significance Level

#### Nonparametric Statistics

95% CLT UCL 0.271
95% Jackknife UCL 0.292
95% Standard Bootstrap UCL 0.262
95% Bootstrap-t UCL 0.446
95% Hall's Bootstrap UCL 1.042
95% Percentile Bootstrap UCL 0.267
95% BCA Bootstrap UCL 0.27
95% Chebyshev(Mean, Sd) UCL 0.422
97.5% Chebyshev(Mean, Sd) UCL 0.527
99% Chebyshev(Mean, Sd) UCL 0.733

Use 95% Student's-t UCL 0.292

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

SS\_Iron

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics** Log-transformed Statistics

Minimum of Log Data 7.719 Minimum 2250 Maximum 13000 Maximum of Log Data 9.473 Mean 5643 Mean of log Data 8.451 Geometric Mean 4681 SD of log Data 0.655 Median 4465 SD 4013 Std. Error of Mean 1638 Coefficient of Variation 0.711

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods! If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.852	Shapiro Wilk Test Statistic 0.96
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788
Data appear Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level

#### **Assuming Normal Distribution**

95% Student's-t UCL 8945 95% H-UCL 14126 95% UCLs (Adjusted for Skewness) 95% Chebyshev (MVUE) UCL 12038 95% Adjusted-CLT UCL (Chen-1995) 9425 97.5% Chebyshev (MVUE) UCL 14836 95% Modified-t UCL (Johnson-1978) 9114 99% Chebyshev (MVUE) UCL 20331

Assuming Lognormal Distribution

97.5% Chebyshev(Mean, Sd) UCL 15875 99% Chebyshev(Mean, Sd) UCL 21945

#### Gamma Distribution Test

**Data Distribution** k star (bias corrected) 1.527 Data appear Normal at 5% Significance Level Theta Star 3697 MLE of Mean 5643 MLE of Standard Deviation 4567 nu star 18.32 Approximate Chi Square Value (.05) 9.622 Nonparametric Statistics Adjusted Level of Significance 0.0122 95% CLT UCL 8338 95% Jackknife UCL 8945

Adjusted Chi Square Value 7.458 95% Standard Bootstrap UCL 8112 Anderson-Darling Test Statistic 0.271 95% Bootstrap-t UCL 12242 Anderson-Darling 5% Critical Value 0.702 95% Hall's Bootstrap UCL 21240 Kolmogorov-Smirnov Test Statistic 0.167 95% Percentile Bootstrap UCL 8363 Kolmogorov-Smirnov 5% Critical Value 0.335 95% BCA Bootstrap UCL 8973 Data appear Gamma Distributed at 5% Significance Level 95% Chebyshev(Mean, Sd) UCL 12785

#### **Assuming Gamma Distribution**

95% Approximate Gamma UCL (Use when n >= 40) 10744 95% Adjusted Gamma UCL (Use when n < 40) 13863

> Potential UCL to Use Use 95% Student's-t UCL 8945

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

SS\_Lead

#### **General Statistics**

Number of Valid Observations 6 Number of Distinct Observations 6

**Raw Statistics** Log-transformed Statistics Minimum of Log Data 2.152 Minimum 8.6 Maximum 43 Maximum of Log Data 3.761 Mean 16.9 Mean of log Data 2.666

Geometric Mean 14.38 Median 12.55 SD 12.89 Std. Error of Mean 5.262

Coefficient of Variation 0.763

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods! If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.615 Shapiro Wilk Test Statistic 0.741 Shapiro Wilk Critical Value 0.788 Shapiro Wilk Critical Value 0.788

Data not Normal at 5% Significance Level Data not Lognormal at 5% Significance Level

#### Assuming Lognormal Distribution Assuming Normal Distribution

95% Student's-t UCL 27.5 95% H-UCL 33.65 95% UCLs (Adjusted for Skewness) 95% Chebyshev (MVUE) UCL 32.53 95% Adjusted-CLT UCL (Chen-1995) 30.97 97.5% Chebyshev (MVUE) UCL 39.54 95% Modified-t UCL (Johnson-1978) 28.35 99% Chebyshev (MVUE) UCL 53.3

#### Gamma Distribution Test **Data Distribution**

k star (bias corrected) 1.738 Data do not follow a Discernable Distribution (0.05)

Theta Star 9.722 MLE of Mean 16.9

MLE of Standard Deviation 12.82 nu star 20.86

Approximate Chi Square Value (.05) 11.49 Adjusted Level of Significance 0.0122

Adjusted Chi Square Value 9.083

Anderson-Darling Test Statistic 1.043 Anderson-Darling 5% Critical Value 0.701 Kolmogorov-Smirnov Test Statistic 0.433 Kolmogorov-Smirnov 5% Critical Value 0.334 Data not Gamma Distributed at 5% Significance Level

**Assuming Gamma Distribution** 95% Approximate Gamma UCL (Use when n >= 40) 30.69 95% Adjusted Gamma UCL (Use when n < 40) 38.81

Potential UCL to Use

## Nonparametric Statistics

95% CLT UCL 25.56 95% Jackknife UCL 27.5 95% Standard Bootstrap UCL 24.8 95% Bootstrap-t UCL 109.3 95% Hall's Bootstrap UCL 91.33 95% Percentile Bootstrap UCL 27.02 95% BCA Bootstrap UCL 27.87 95% Chebyshev(Mean, Sd) UCL 39.84 97.5% Chebyshev(Mean, Sd) UCL 49.76 99% Chebyshev(Mean, Sd) UCL 69.26

SD of log Data 0.558

Use 95% Chebyshev (Mean, Sd) UCL 39.84

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

#### SS\_Magnesium

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics** Log-transformed Statistics

Minimum of Log Data 7.056 Minimum 1160 Maximum 6010 Maximum of Log Data 8.701 Mean 2618 Mean of log Data 7.731 Geometric Mean 2278 SD of log Data 0.546 Median 2125 SD 1726 Std. Error of Mean 704.7 Coefficient of Variation 0.659

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods! If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test	
Shapiro Wilk Test Statistic 0.751	Shapiro Wilk Test Statistic 0.908	
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788	
Data not Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level	

#### **Assuming Normal Distribution**

95% Student's-t UCL 4038 95% H-UCL 5179 95% UCLs (Adjusted for Skewness) 95% Chebyshev (MVUE) UCL 5071 95% Adjusted-CLT UCL (Chen-1995) 4405 97.5% Chebyshev (MVUE) UCL 6151 95% Modified-t UCL (Johnson-1978) 4136 99% Chebyshev (MVUE) UCL 8274

# Gamma Distribution Test

**Data Distribution** k star (bias corrected) 1.984 Data appear Gamma Distributed at 5% Significance Level Theta Star 1320 MLE of Mean 2618 MLE of Standard Deviation 1859 nu star 23.81 Approximate Chi Square Value (.05) 13.71 Nonparametric Statistics Adjusted Level of Significance 0.0122 95% CLT UCL 3777 Adjusted Chi Square Value 11.04 95% Jackknife UCL 4038 95% Standard Bootstrap UCL 3660 95% Bootstrap-t UCL 6052 95% Hall's Bootstrap UCL 9042

Anderson-Darling Test Statistic 0.526 Anderson-Darling 5% Critical Value 0.7 Kolmogorov-Smirnov Test Statistic 0.309 Kolmogorov-Smirnov 5% Critical Value 0.334 Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 4549 95% Adjusted Gamma UCL (Use when n < 40) 5648

Use 95% Approximate Gamma UCL 4549

95% Percentile Bootstrap UCL 3897

95% Chebyshev(Mean, Sd) UCL 5690 97.5% Chebyshev(Mean, Sd) UCL 7019

99% Chebyshev(Mean, Sd) UCL 9630

95% BCA Bootstrap UCL 4115

Assuming Lognormal Distribution

Potential UCL to Use

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Manganese

#### **General Statistics**

Number of Valid Observations 6

Log-transformed Statistics

Raw Statistics
Minimum 65
Maximum 259
Mean 128.8
Geometric Mean 117.1

Geometric Mean 117.1

Median 107

SD 67.83

Std. Error of Mean 27.69

Coefficient of Variation 0.527

Minimum of Log Data 4.174 Maximum of Log Data 5.557 Mean of log Data 4.763 SD of log Data 0.458

Number of Distinct Observations 6

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.803	Shapiro Wilk Test Statistic 0.924
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788

Data appear Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

Assuming Normal Distribution

95% Student's-t UCL 184.6

95% UCLs (Adjusted for Skewness)
95% Adjusted-CLT UCL (Chen-1995) 196.4
95% Modified-t UCL (Johnson-1978) 188

Assuming Lognormal Distribution

95% H-UCL 219 95% Chebyshev (MVUE) UCL 231.8 97.5% Chebyshev (MVUE) UCL 276.8 99% Chebyshev (MVUE) UCL 365.2

Gamma Distribution Test

k star (bias corrected) 2.824 Theta Star 45.61

MLE of Mean 128.8
MLE of Standard Deviation 76.65
nu star 33.89

Approximate Chi Square Value (.05) 21.57

Adjusted Level of Significance 0.0122

Adjusted Chi Square Value 18.11

Anderson-Darling Test Statistic 0.457
Anderson-Darling 5% Critical Value 0.698
Kolmogorov-Smirnov Test Statistic 0.266
Kolmogorov-Smirnov 5% Critical Value 0.333

Data appear Gamma Distributed at 5% Significance Level

Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 202.3 95% Adjusted Gamma UCL (Use when n < 40) 241

Nonparametric Statistics

**Data Distribution** 

Data appear Normal at 5% Significance Level

95% CLT UCL 174.3
95% Jackknife UCL 184.6
95% Standard Bootstrap UCL 170.2
95% Bootstrap-t UCL 259.7
95% Hall's Bootstrap UCL 445
95% Percentile Bootstrap UCL 175.7
95% BCA Bootstrap UCL 186.6
95% Chebyshev(Mean, Sd) UCL 249.5
97.5% Chebyshev(Mean, Sd) UCL 301.7
99% Chebyshev(Mean, Sd) UCL 404.3

Potential UCL to Use

Use 95% Student's-t UCL 184.6

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

#### SS\_Mercury

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

Log-transformed Statistics

Assuming Lognormal Distribution

**Data Distribution** 

95% H-UCL 1.94

95% Chebyshev (MVUE) UCL 1.196

99% Chebyshev (MVUE) UCL 2.106

97.5% Chebyshev (MVUE) UCL 1.503

v Statistics		
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Minimum of Log Data -2.04 Minimum 0.13 Maximum 1.5 Maximum of Log Data 0.405 Mean 0.507 Mean of log Data -0.995 Geometric Mean 0.37 SD of log Data 0.827 Median 0.35 SD 0.503 Std. Error of Mean 0.205 Coefficient of Variation 0.992

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods! If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.729	Shapiro Wilk Test Statistic 0.95
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788
Data not Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level

#### **Assuming Normal Distribution**

95% Student's-t UCL 0.92 95% UCLs (Adjusted for Skewness) 95% Adjusted-CLT UCL (Chen-1995) 1.033 95% Modified-t UCL (Johnson-1978) 0.95

# Gamma Distribution Test

k star (bias corrected) 0.978 Data appear Gamma Distributed at 5% Significance Level Theta Star 0.518 MLE of Mean 0.507 MLE of Standard Deviation 0.512 nu star 11.74 Approximate Chi Square Value (.05) 5.057 Nonparametric Statistics Adjusted Level of Significance 0.0122 95% CLT UCL 0.844 Adjusted Chi Square Value 3.597 95% Jackknife UCL 0.92 95% Standard Bootstrap UCL 0.812 Anderson-Darling Test Statistic 0.433 95% Bootstrap-t UCL 1.688 Anderson-Darling 5% Critical Value 0.706 95% Hall's Bootstrap UCL 2.22 Kolmogorov-Smirnov Test Statistic 0.27 95% Percentile Bootstrap UCL 0.883 Kolmogorov-Smirnov 5% Critical Value 0.337 95% BCA Bootstrap UCL 0.945 Data appear Gamma Distributed at 5% Significance Level 95% Chebyshev(Mean, Sd) UCL 1,401 97.5% Chebyshev(Mean, Sd) UCL 1.788 99% Chebyshev(Mean, Sd) UCL 2.548

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 1.176 95% Adjusted Gamma UCL (Use when n < 40) 1.654

#### Potential UCL to Use

Use 95% Approximate Gamma UCL 1.176

#### **User Selected Options**

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Number of Bootstrap Operations 10000

#### SS Nickel

#### **General Statistics**

Number of Valid Observations 6 Number of Distinct Observations 5

Raw Statistics	Log-transformed Statistics
Minimum 1.7	Minimum of Log Data 0.531
Maximum 18.5	Maximum of Log Data 2.918
Mean 6.783	Mean of log Data 1.46

SD of log Data 1.011

Geometric Mean 4.304 Median 2.6 SD 7.168 Std. Error of Mean 2.926 Coefficient of Variation 1 057

Skewness 1.206

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methodsl If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.742	Shapiro Wilk Test Statistic 0.799
Shaniro Wilk Critical Value 0 788	Shaniro Wilk Critical Value 0 788

Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

#### Assuming Normal Distribution Assuming Lognormal Distribution 95% Student's-t UCL 12.68 95% H-UCL 47.22 95% UCLs (Adjusted for Skewness) 95% Chebyshev (MVUE) UCL 17.83

95% Adjusted-CLT UCL (Chen-1995) 13.14 97.5% Chebyshev (MVUE) UCL 22.75 95% Modified-t UCL (Johnson-1978) 12.92 99% Chebyshev (MVUE) UCL 32.43

#### **Gamma Distribution Test Data Distribution**

k star (bias corrected) 0.731	Data appear Lognormal at 5% Significance Level
Thota Star 0 292	

MLF of Mean 6 783

MLE of Standard Deviation 7.935

nu star 8.769

Approximate Chi Square Value (.05) 3.188 Nonparametric Statistics 95% CLT UCL 11.6

Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 2.102 95% Jackknife UCL 12.68 95% Standard Bootstrap UCL 11.16 Anderson-Darling Test Statistic 0.806 95% Bootstrap-t UCL 86.93

Anderson-Darling 5% Critical Value 0.712 95% Hall's Bootstrap UCL 96.63 Kolmogorov-Smirnov Test Statistic 0.393 95% Percentile Bootstrap UCL 11.37 Kolmogorov-Smirnov 5% Critical Value 0.339 95% BCA Bootstrap UCL 12.13 Data not Gamma Distributed at 5% Significance Level 95% Chebyshev(Mean, Sd) UCL 19.54 97.5% Chebyshev(Mean, Sd) UCL 25.06

95% Adjusted Gamma UCL (Use when n < 40) 28.3

Assuming Gamma Distribution 99% Chebyshev(Mean, Sd) UCL 35.9 95% Approximate Gamma UCL (Use when n >= 40) 18.66

> Potential UCL to Use Use 95% Chebyshev (Mean, Sd) UCL 19.54

Recommended UCL exceeds the maximum observation

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

#### SS\_Phenanthrene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### **Raw Statistics**

Minimum 0.043 Maximum 0.35 Mean 0.142 Geometric Mean 0.106 Median 0.0905 SD 0.122

SD 0.122 Std. Error of Mean 0.0499 Coefficient of Variation 0.86 Skewness 1.246

#### Log-transformed Statistics

Minimum of Log Data -3.147 Maximum of Log Data -1.05 Mean of log Data -2.248 SD of log Data 0.835

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesl

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

### Relevant UCL Statistics

Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.826	Shapiro Wilk Test Statistic 0.914
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788
Data appear Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level

#### Assuming Normal Distribution

95% Student's-t UCL 0.243

95% UCLs (Adjusted for Skewness)

95% Adjusted-CLT UCL (Chen-1995) 0.251

95% Modified-t UCL (Johnson-1978) 0.247

#### Assuming Lognormal Distribution

95% H-UCL 0.57 95% Chebyshev (MVUE) UCL 0.345 97.5% Chebyshev (MVUE) UCL 0.434 99% Chebyshev (MVUE) UCL 0.609

#### Gamma Distribution Test

Theta Star 0.138

MLE of Mean 0.142

MLE of Standard Deviation 0.14

k star (bias corrected) 1.027

nu star 12.33 Approximate Chi Square Value (.05) 5.442

Adjusted Level of Significance 0.0122 Adjusted Chi Square Value 3.913

Anderson-Darling Test Statistic 0.416
Anderson-Darling 5% Critical Value 0.705
Kolmogorov-Smirnov Test Statistic 0.282
Kolmogorov-Smirnov 5% Critical Value 0.336

Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 0.322 95% Adjusted Gamma UCL (Use when n < 40) 0.448

# Data Distribution

Data appear Normal at 5% Significance Level

#### Nonparametric Statistics

95% Jackknife UCL 0.243
95% Standard Bootstrap UCL 0.217
95% Bootstrap-t UCL 0.522
95% Hall's Bootstrap UCL 0.857
95% Percentile Bootstrap UCL 0.223
95% BCA Bootstrap UCL 0.237
95% Chebyshev(Mean, Sd) UCL 0.36
97.5% Chebyshev(Mean, Sd) UCL 0.454
99% Chebyshev(Mean, Sd) UCL 0.639

95% CLT UCL 0.224

#### Potential UCL to Use

Use 95% Student's-t UCL 0.243

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Potassium

#### **General Statistics**

Number of Valid Observations 6 Number of Distinct Observations 6

Raw Statistics		Log-transformed Statistics
Minimum	605	Minimum of Log Data 6.405
Maximum	4000	Maximum of Log Data 8.294
Mean	1326	Mean of log Data 6.937
Geometric Mean	1029	SD of log Data 0.678
Median	846	
SD	1313	
Std. Error of Mean	536.2	
Coefficient of Variation	0.991	
Skewness	2.42	

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

	•	•	
	Relevant UCL Stati	stics	
Normal Distribution Test		Lognormal Distribution Test	
Shapiro Wilk Test Statistic	0.56	Shapiro Wilk Test Statistic 0.6	61
Shapiro Wilk Critical Value	0.788	Shapiro Wilk Critical Value 0.7	/88
Data not Normal at 5% Significance Level		Data not Lognormal at 5% Significance Level	
Assuming Normal Distribution		Assuming Lognormal Distribution	
95% Student's-t UCL	2406	95% H-UCL 33	23
95% UCLs (Adjusted for Skewness)		95% Chebyshev (MVUE) UCL 27	30
95% Adjusted-CLT UCL (Chen-1995)	2774	97.5% Chebyshev (MVUE) UCL 33	75
95% Modified-t UCL (Johnson-1978)	2495	99% Chebyshev (MVUE) UCL 46	42
Gamma Distribution Test		Data Distribution	
k star (bias corrected)	1.174	Data do not follow a Discernable Distribution (0.05)	
Theta Star	1129		
MLE of Mean	1326		
MLE of Standard Deviation	1223		
nu star	14.09		
Approximate Chi Square Value (.05)	6.635	Nonparametric Statistics	
Adjusted Level of Significance	0.0122	95% CLT UCL 22	80
Adjusted Chi Square Value	4.907	95% Jackknife UCL 24	06
		95% Standard Bootstrap UCL 21	24
Anderson-Darling Test Statistic	1.296	95% Bootstrap-t UCL 32	836
Anderson-Darling 5% Critical Value	0.704	95% Hall's Bootstrap UCL 18	743
Kolmogorov-Smirnov Test Statistic	0.474	95% Percentile Bootstrap UCL 23	77
Kolmogorov-Smirnov 5% Critical Value	0.336	95% BCA Bootstrap UCL 24	22
Data not Gamma Distributed at 5% Significance Le	evel	95% Chebyshev(Mean, Sd) UCL 36	63
		97.5% Chebyshev(Mean, Sd) UCL 46	75
Assuming Gamma Distribution		99% Chebyshev(Mean, Sd) UCL 66	61

Potential UCL to Use Use 95% Chebyshev (Mean, Sd) UCL 3663

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Singh, and Iacl (2002) and Singh and Singh (2003). For additional insight, the user may want to consult a statistician.

95% Approximate Gamma UCL (Use when n >= 40) 2816 95% Adjusted Gamma UCL (Use when n < 40) 3808

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Pyrene

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### Raw Statistics

# Minimum 0.12 Maximum 1.1 Mean 0.398 Geometric Mean 0.267 Median 0.17 SD 0.407

# Log-transformed Statistics Minimum of Log Data -2.12 Maximum of Log Data 0.0953 Mean of log Data -1.32

SD of log Data 0.939

Std. Error of Mean 0.166 Coefficient of Variation 1.021 Skewness 1.37

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

Normal Distribution 1980	Lognormal Distribution Test	
Shapiro Wilk Test Statistic 0.751	Shapiro Wilk Test Statistic 0.813	
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788	
Data not Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level	
Assuming Normal Distribution	Assuming Lognormal Distribution	

#### Assuming Normal Distribution 95% Student's-t UCL 0.733

Normal Distribution Tost

95% UCLs (Adjusted for Skewness)	
95% Adjusted-CLT UCL (Chen-1995) 0.771	
95% Modified-t UCL (Johnson-1978) 0.748	

#### Assuming Lognormal Distribution

Lognormal Distribution Tost

95% H-UCL 2.138 95% Chebyshev (MVUE) UCL 1.004 97.5% Chebyshev (MVUE) UCL 1.275 99% Chebyshev (MVUE) UCL 1.806

#### Gamma Distribution Test k star (bias corrected) 0.808

0.493	Theta Star
0.398	MLE of Mean
0.443	MLE of Standard Deviation
9.701	nu star
3.756	Approximate Chi Square Value (.05)

# Nonparametric Statistics

Data Distribution

Data appear Lognormal at 5% Significance Level

Adjusted Level of Significance 0.0122	95% CLT UCL 0.671
Adjusted Chi Square Value 2.548	95% Jackknife UCL 0.733
	95% Standard Bootstrap UCL 0.646
Anderson-Darling Test Statistic 0.73	95% Bootstrap-t UCL 4.209
Anderson-Darling 5% Critical Value 0.709	95% Hall's Bootstrap UCL 3.633
Kolmogorov-Smirnov Test Statistic 0.351	95% Percentile Bootstrap UCL 0.652
Kolmogorov-Smirnov 5% Critical Value 0.338	95% BCA Bootstrap UCL 0.72
amma Distributed at 5% Significance Level	95% Chebyshev(Mean, Sd) UCL 1.122
	97.5% Chehyshey(Mean, Sd) UCL 1.435

# Assuming Gamma Distribution

Data not Gamma Distrib

95% Approximate Gamma UCL (Use when n >= 40) 1.029 95% Adjusted Gamma UCL (Use when n < 40) 1.517

Use 95% H-UCL 2.138

99% Chebyshev(Mean, Sd) UCL 2.05

# Potential UCL to Use Recommended UCL exceeds the maximum observation

ProUCL computes and outputs H-statistic based UCLs for historical reasons only.

H-statistic often results in unstable (both high and low) values of UCL95 as shown in examples in the Technical Guide.

It is therefore recommended to avoid the use of H-statistic based 95% UCLs.

Use of nonparametric methods are preferred to compute UCL95 for skewed data sets which do not follow a gamma distribution.

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Sodium

		General Statistics	
5	Number of Detected Data	6	Number of Valid Data
1	Number of Non-Detect Data	5	Number of Distinct Detected Data
16.67%	Percent Non-Detects		
	Log-transformed Statistics		Raw Statistics
6.438	Minimum Detected	625	Minimum Detected
8.35	Maximum Detected	4230	Maximum Detected
7.347	Mean of Detected	1935	Mean of Detected
0.747	SD of Detected	1442	SD of Detected
6.107	Minimum Non-Detect	449	Minimum Non-Detect
6 107	Maximum Non-Detect	449	Maximum Non-Detect

Warning: There are only 5 Detected Values in this data

Note: It should be noted that even though bootstrap may be performed on this data set
the resulting calculations may not be reliable enough to draw conclusions

It is recommended to have 10-15 or more distinct observations for accurate and meaningful results.

ly	Lognormal Distribution Test with Detected Values On	he.
		/y
0.898	Shapiro Wilk Test Statistic	0.989
0.762	5% Shapiro Wilk Critical Value	0.762
	Data appear Lognormal at 5% Significance Level	
	Assuming Lognormal Distribution	
	DL/2 Substitution Method	
1650	Mean	7.025
1467	SD	1.03
2856	95% H-Stat (DL/2) UCL	13675
	Log ROS Method	
1541	Mean in Log Scale	7.02
1500	SD in Log Scale	1.043
2775	Mean in Original Scale	1649
2773	SD in Original Scale	1468
	95% t UCL	2856
	95% Percentile Bootstrap UCL	2610
	95% BCA Bootstrap UCL	279
	95% H UCL	14169
ly	Data Distribution Test with Detected Values Only	
1.101	Data appear Normal at 5% Significance Level	
1757		
11.01		
0.21	Nonparametric Statistics	
0.684	Kaplan-Meier (KM) Method	
0.684	Mean	1717
0.36	SD	1275
.evel	SE of Mean	581.9
	95% KM (t) UCL	2889
	95% KM (z) UCL	2674
	95% KM (jackknife) UCL	2857
0.000001	95% KM (bootstrap t) UCL	4350
4230	95% KM (BCA) UCL	2763
1612	95% KM (Percentile Bootstrap) UCL	2690
1220	95% KM (Chebyshev) UCL	4253
1513	97.5% KM (Chebyshev) UCL	5350
0.214	99% KM (Chebyshev) UCL	7506
7539		
2.566	Potential UCLs to Use	
0.256	95% KM (t) UCL	2889
16133	95% KM (Percentile Bootstrap) UCL	2690
	0.762  1650 1467 2856  1541 1500 2775 2773  1.101 1757 11.01 0.21 0.684 0.36  0.000001 4230 1612 1220 1513 0.214 7539 2.566	Data appear Lognormal at 5% Significance Level

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

### SS\_TOTAL HPAH

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

aw Statistics		Log-transformed Statistics	
Minimum	0.676	Minimum of Log Data	-0.392
Maximum	5.866	Maximum of Log Data	1.769
Mean	2.491	Mean of log Data	0.57
Geometric Mean	1.768	SD of log Data	0.896
Median	1.329		
SD	2.248		
Std. Error of Mean	0.918		
Coefficient of Variation	0.903		
Skewness	0.992		

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

	Relevant	UCL Statistics
Normal Distribution Test		Lognormal Distribution Test
Shapiro Wilk Test Statistic	0.789	Shapiro Wilk Test Statistic 0.88
Shapiro Wilk Critical Value	0.788	Shapiro Wilk Critical Value 0.788
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level
Assuming Normal Distribution		Assuming Lognormal Distribution
95% Student's-t UCL	4.34	95% H-UCL 11.91
95% UCLs (Adjusted for Skewness)		95% Chebyshev (MVUE) UCL 6.273
95% Adjusted-CLT UCL (Chen-1995)	4.398	97.5% Chebyshev (MVUE) UCL 7.934
95% Modified-t UCL (Johnson-1978)	4.402	99% Chebyshev (MVUE) UCL 11.2
Gamma Distribution Test		Data Distribution
k star (bias corrected)	0.914	Data appear Normal at 5% Significance Level
Theta Star	2.726	
MLE of Mean	2.491	
MLE of Standard Deviation	2.606	
nu star	10.96	
Approximate Chi Square Value (.05)	4.552	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 4
Adjusted Chi Square Value	3.185	95% Jackknife UCL 4.34
		95% Standard Bootstrap UCL 3.873
Anderson-Darling Test Statistic	0.55	95% Bootstrap-t UCL 12.23
Anderson-Darling 5% Critical Value	0.707	95% Hall's Bootstrap UCL 16.46
Kolmogorov-Smirnov Test Statistic	0.271	95% Percentile Bootstrap UCL 3.976
Kolmogorov-Smirnov 5% Critical Value	0.337	95% BCA Bootstrap UCL 4.082
Data appear Gamma Distributed at 5% Significance	Level	95% Chebyshev(Mean, Sd) UCL 6.491
		97.5% Chebyshev(Mean, Sd) UCL 8.222
Assuming Gamma Distribution		99% Chebyshev(Mean, Sd) UCL 11.62
95% Approximate Gamma UCL (Use when n >= 40)	5.998	

Potential UCL to Use Use 95% Student's-t UCL 4.34

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Singh, and Iacl (2002) and Singh and Singh (2003). For additional insight, the user may want to consult a statistician.

95% Adjusted Gamma UCL (Use when n < 40) 8.572

#### **User Selected Options**

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

### SS\_TOTAL LPAH

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

Raw Statistics		Log-transformed Statistics
Minimum	0.069	Minimum of Log Data -2.674
Maximum	0.449	Maximum of Log Data -0.801
Mean	0.205	Mean of log Data -1.866
Geometric Mean	0.155	SD of log Data 0.815
Median	0.123	
SD	0.169	
Std. Error of Mean	0.0689	
Coefficient of Variation	0.822	
Skewness	0.906	

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

	Relevant UCI	L Statistics
Normal Distribution Test		Lognormal Distribution Test
Shapiro Wilk Test Statistic	0.792	Shapiro Wilk Test Statistic 0.858
Shapiro Wilk Critical Value	0.788	Shapiro Wilk Critical Value 0.788
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level
Assuming Normal Distribution		Assuming Lognormal Distribution
95% Student's-t UCL	0.344	95% H-UCL 0.778
95% UCLs (Adjusted for Skewness)		95% Chebyshev (MVUE) UCL 0.492
95% Adjusted-CLT UCL (Chen-1995)	0.346	97.5% Chebyshev (MVUE) UCL 0.618
95% Modified-t UCL (Johnson-1978)	0.348	99% Chebyshev (MVUE) UCL 0.865
Gamma Distribution Test		Data Distribution
k star (bias corrected)	1.069	Data appear Normal at 5% Significance Level
Theta Star	0.192	
MLE of Mean	0.205	
MLE of Standard Deviation	0.199	
nu star	12.83	
Approximate Chi Square Value (.05)	5.78	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 0.319
Adjusted Chi Square Value	4.192	95% Jackknife UCL 0.344
		95% Standard Bootstrap UCL 0.309
Anderson-Darling Test Statistic	0.566	95% Bootstrap-t UCL 0.676
Anderson-Darling 5% Critical Value	0.705	95% Hall's Bootstrap UCL 1.269
Kolmogorov-Smirnov Test Statistic	0.266	95% Percentile Bootstrap UCL 0.316
Kolmogorov-Smirnov 5% Critical Value	0.336	95% BCA Bootstrap UCL 0.326
Data appear Gamma Distributed at 5% Significance	Level	95% Chebyshev(Mean, Sd) UCL 0.506
		97.5% Chebyshev(Mean, Sd) UCL 0.636
Assuming Gamma Distribution		99% Chebyshev(Mean, Sd) UCL 0.891
95% Approximate Gamma UCL (Use when n >= 40)	0.456	
95% Adjusted Gamma UCL (Use when n < 40)	0.629	

Potential UCL to Use Use 95% Student's-t UCL 0.344

#### User Selected Options

#### SS\_Trichlorofluoromethane

	General S	Statistics	
Number of Valid Data	6	Number of Detected Data	4
Number of Distinct Detected Data	4	Number of Non-Detect Data	2
		Percent Non-Detects	33.33%
Raw Statistics		Log-transformed Statistics	
Minimum Detected	0.00023	Minimum Detected	-8.377
Maximum Detected	0.0005	Maximum Detected	-7.601
Mean of Detected	0.0003125	Mean of Detected	-8.122
SD of Detected	0.0001261	SD of Detected	0.354
Minimum Non-Detect	0.0049	Minimum Non-Detect	-5.319
Maximum Non-Detect	0.0051	Maximum Non-Detect	-5.279
Note: Data have multiple DLs - Use of KM Method is recomme	nded	Number treated as Non-Detect	6
For all methods (except KM, DL/2, and ROS Methods),		Number treated as Detected	0
Observations < Largest ND are treated as NDs		Single DL Non-Detect Percentage	100.00%

Warning: There are only 4 Distinct Detected Values in this data

Note: It should be noted that even though bootstrap may be performed on this data set
the resulting calculations may not be reliable enough to draw conclusions

It is recommended to have 10-15 or more distinct observations for accurate and meaningful results.

	UCL St	atistics	
Normal Distribution Test with Detected Values Or	nly	Lognormal Distribution Test with Detected Values C	Only
Shapiro Wilk Test Statistic	0.748	Shapiro Wilk Test Statistic	0.796
5% Shapiro Wilk Critical Value	0.748	5% Shapiro Wilk Critical Value	0.748
Data appear Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Leve	ıl
Assuming Normal Distribution		Assuming Lognormal Distribution	
DL/2 Substitution Method		DL/2 Substitution Method	
Mean	0.00104	Mean	-7.412
SD	0.00113	SD	1.134
95% DL/2 (t) UCL	0.00197	95% H-Stat (DL/2) UCL	0.0118
Maximum Likelihood Estimate(MLE) Method	N/A	Log ROS Method	
MLE method failed to converge properly		Mean in Log Scale	-8.122
		SD in Log Scale	0.274
		Mean in Original Scale	0.0003073
		SD in Original Scale	9.798E-05
		95% t UCL	0.0003879
		95% Percentile Bootstrap UCL	0.0003783
		95% BCA Bootstrap UCL	0.0003873
		95% H-UCL	0.0004027
Gamma Distribution Test with Detected Values O	nly	Data Distribution Test with Detected Values Only	,
k star (bias corrected)	2.637	Data appear Normal at 5% Significance Level	
Theta Star	0.0001185		
nu star	21.09		
A-D Test Statistic	0.619	Nonparametric Statistics	
5% A-D Critical Value	0.657	Kaplan-Meier (KM) Method	
K-S Test Statistic	0.657	Mean	0.0003125
5% K-S Critical Value	0.395	SD	0.0001092
ata appear Gamma Distributed at 5% Significance	Level	SE of Mean	6.303E-05
		95% KM (t) UCL	0.0004395
Assuming Gamma Distribution		95% KM (z) UCL	0.0004162
Gamma ROS Statistics using Extrapolated Data		95% KM (jackknife) UCL	0.0004464
Minimum	0.00023	95% KM (bootstrap t) UCL	0.00104
Maximum	0.0005	95% KM (BCA) UCL	0.0004167
Mean	0.0003154	95% KM (Percentile Bootstrap) UCL	0.0004167
Median	0.0002956	95% KM (Chebyshev) UCL	0.0005873
SD	9.775E-05	97.5% KM (Chebyshev) UCL	0.0007061
k star	7.463	99% KM (Chebyshev) UCL	0.0009397
Theta star	4.226E-05		
Nu star	89.55	Potential UCLs to Use	
AppChi2	68.73	95% KM (t) UCL	0.0004395
95% Gamma Approximate UCL (Use when n >= 40)	0.0004109	95% KM (Percentile Bootstrap) UCL	0.0004167
95% Adjusted Commo LICL (Lice when n < 40)	NI/A		

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

These recommendations are based upon the results of the simulation studies summarized in Singh, Malchle, and Lee (2006).

For additional insight, the user may want to consult a statistician.

95% Adjusted Gamma UCL (Use when n < 40) N/A

Note: DL/2 is not a recommended method.

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

#### SS\_Vanadium

#### **General Statistics**

Number of Valid Observations 6

Number of Distinct Observations 6

#### Raw Statistics

Minimum 3.4 Maximum 21.3 Mean 8.1 Geometric Mean 6.692 Median 6

SD 6.578 Std. Error of Mean 2.685 Coefficient of Variation 0.812 Skewness 2.261

#### Log-transformed Statistics

Minimum of Log Data 1.224 Maximum of Log Data 3.059 Mean of log Data 1.901 SD of log Data 0.618

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimates!

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

#### Relevant UCL Statistics

TOTALL GGZ GLABOUG	
Normal Distribution Test	Lognormal Distribution Test
Shapiro Wilk Test Statistic 0.674	Shapiro Wilk Test Statistic 0.851
Shapiro Wilk Critical Value 0.788	Shapiro Wilk Critical Value 0.788
Data not Normal at 5% Significance Level	Data appear Lognormal at 5% Significance Level

# Assuming Normal Distribution Assuming Lognormal Distribution 95% Student's-t UCL 13.51 95% I

 95% Student's-t UCL 13.51
 95% H-UCL 18.28

 95% UCLs (Adjusted for Skewness)
 95% Chebyshev (MVUE) UCL 16.4

 95% Adjusted-CLT UCL (Chen-1995) 15.17
 97.5% Chebyshev (MVUE) UCL 20.11

 95% Modified-t UCL (Johnson-1978) 13.92
 99% Chebyshev (MVUE) UCL 27.41

#### Gamma Distribution Test

Theta Star 5.408 MLE of Mean 8.1 MLE of Standard Deviation 6.619 nu star 17.97

k star (bias corrected) 1.498

Approximate Chi Square Value (.05) 9.371

Adjusted Level of Significance 0.0122

Adjusted Chi Square Value 7.24

Anderson-Darling Test Statistic 0.728
Anderson-Darling 5% Critical Value 0.702
Kolmogorov-Smirnov Test Statistic 0.365
Kolmogorov-Smirnov 5% Critical Value 0.335
Data not Gamma Distributed at 5% Significance Level

# Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 15.53 95% Adjusted Gamma UCL (Use when n < 40) 20.11

# Data Distribution

Data appear Lognormal at 5% Significance Level

### Nonparametric Statistics

95% CLT UCL 12.52
95% Jackknife UCL 13.51
95% Standard Bootstrap UCL 12.13
95% Bootstrap+t UCL 28.73
95% Hall's Bootstrap UCL 35.9
95% Percentile Bootstrap UCL 13.2
95% BCA Bootstrap UCL 13.83
95% Chebyshev(Mean, Sd) UCL 19.81
97.5% Chebyshev(Mean, Sd) UCL 24.87
99% Chebyshev(Mean, Sd) UCL 34.82

#### Potential UCL to Use

Use 95% H-UCL 18.28

ProUCL computes and outputs H-statistic based UCLs for historical reasons only.

H-statistic often results in unstable (both high and low) values of UCL95 as shown in examples in the Technical Guide.

It is therefore recommended to avoid the use of H-statistic based 95% UCLs.

Use of nonparametric methods are preferred to compute UCL95 for skewed data sets which do not follow a gamma distribution.

#### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Number of Bootstrap Operations
 10000

SS\_Zinc

#### **General Statistics**

Number of Valid Observations 6 Number of Distinct Observations 6

Raw Statistics	Log-transformed Statistics
Minimum 71.8	Minimum of Log Data 4.274
Maximum 560	Maximum of Log Data 6.328
Mean 203.1	Mean of log Data 5.058
Geometric Mean 157.2	SD of log Data 0.732
Median 128	
SD 183	
Std. Error of Mean 74.72	

Warning: A sample size of 'n' = 6 may not adequate enough to compute meaningful and reliable test statistics and estimatesi

Coefficient of Variation 0.901 Skewness 2.019

It is suggested to collect at least 8 to 10 observations using these statistical methods!

If possible compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

#### Warning: There are only 6 Values in this data

Note: It should be noted that even though bootstrap methods may be performed on this data set, the resulting calculations may not be reliable enough to draw conclusions

The literature suggests to use bootstrap methods on data sets having more than 10-15 observations.

	Relevant	UCL Statistics
Normal Distribution Test		Lognormal Distribution Test
Shapiro Wilk Test Statistic	0.74	Shapiro Wilk Test Statistic 0.917
Shapiro Wilk Critical Value	0.788	Shapiro Wilk Critical Value 0.788
Data not Normal at 5% Significance Level		Data appear Lognormal at 5% Significance Level
Assuming Normal Distribution		Assuming Lognormal Distribution
95% Student's-t UCL	353.6	95% H-UCL 598.1
95% UCLs (Adjusted for Skewness)		95% Chebyshev (MVUE) UCL 447.9
95% Adjusted-CLT UCL (Chen-1995)	391.8	97.5% Chebyshev (MVUE) UCL 557.3
95% Modified-t UCL (Johnson-1978)	363.9	99% Chebyshev (MVUE) UCL 772.1
Gamma Distribution Test		Data Distribution
k star (bias corrected)	1.164	Data appear Gamma Distributed at 5% Significance Level
Theta Star	174.4	
MLE of Mean	203.1	
MLE of Standard Deviation	188.2	
nu star	13.97	
Approximate Chi Square Value (.05)	6.551	Nonparametric Statistics
Adjusted Level of Significance	0.0122	95% CLT UCL 326
Adjusted Chi Square Value	4.836	95% Jackknife UCL 353.6
		95% Standard Bootstrap UCL 315.9
Anderson-Darling Test Statistic	0.494	95% Bootstrap-t UCL 943.6
Anderson-Darling 5% Critical Value	0.704	95% Hall's Bootstrap UCL 1058
Kolmogorov-Smirnov Test Statistic	0.291	95% Percentile Bootstrap UCL 332.3
Kolmogorov-Smirnov 5% Critical Value	0.336	95% BCA Bootstrap UCL 377.2

Potential UCL to Use

Assuming Gamma Distribution

95% Approximate Gamma UCL (Use when n >= 40) 433

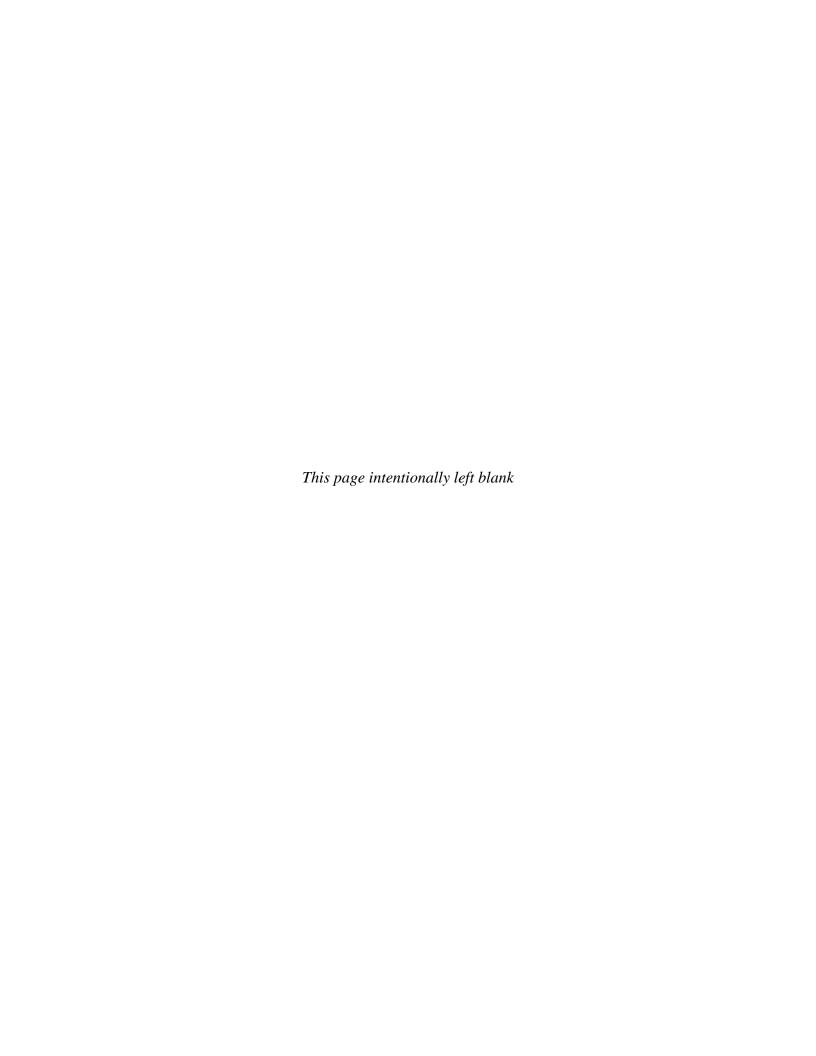
95% Adjusted Gamma UCL (Use when n < 40) 586.6

Use 95% Approximate Gamma UCL 433

97.5% Chebyshev(Mean, Sd) UCL 669.7 99% Chebyshev(Mean, Sd) UCL 946.5

# **APPENDIX C-2**

# ProUCL STATISTICAL DATA OUTPUT – BACKGROUND DATA FOR CHEMICALS OF POTENTIAL ECOLOGICAL CONCERN



### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Coverage
 90%

 Different or Future K Values
 1

Different or Future K Values 1

Number of Bootstrap Operations 2000

#### SS\_Barium

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 14

Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statistics
----------------	----------------------------

Minimum 19.6 Minimum 2.976 Maximum 1520 Maximum 7.326 Second Largest 1070 Second Largest 6.975 First Quartile 30.95 First Quartile 3.43 Median 4.745 Median 115 Third Quartile 288 Third Quartile 5.642 Mean 291.5 Mean 4.697 Geometric Mean 109.6 SD 1.46

SD 441.2 Coefficient of Variation 1.514

Skewness 2.118

### **Background Statistics**

#### Normal Distribution Test Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.67 Shapiro Wilk Test Statistic 0.912 Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

# Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

#### Assuming Normal Distribution Assuming Lognormal Distribution

95% UTL with 90% Coverage 1204 95% UTL with 90% Coverage 2244 95% UPL (t) 1094 95% UPL (t) 1560 90% Percentile (z) 856.9 90% Percentile (z) 711.8 95% Percentile (z) 1017 95% Percentile (z) 1210 99% Percentile (z) 1318 99% Percentile (z) 3272

# Gamma Distribution Test Data Distribution Test

k star 0.546 **Data appear Gamma Distributed at 5% Significance Level**Theta Star 533.5
MLE of Mean 291.5

MLE of Standard Deviation 394.4 nu star 16.39

A-D Test Statistic 0.783 Nonparametric Statistics

5% A-D Critical Value 0.784 90% Percentile 859.2
K-S Test Statistic 0.225 95% Percentile 1205
5% K-S Critical Value 0.232 99% Percentile 1457

#### Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution 95% UTL with 90% Coverage 1520

 90% Percentile 774
 95% Percentile Bootstrap UTL with
 90% Coverage 1520

 95% Percentile 1085
 95% BCA Bootstrap UTL with
 90% Coverage 1520

 99% Percentile 1843
 95% UPL 1520

 95% Chebyshev UPL 2278

95% WH Approx. Gamma UPL 1145 Upper Threshold Limit Based upon IQR 673.6

95% HW Approx. Gamma UPL 1193

95% WH Approx. Gamma UTL with 90% Coverage 1389

95% HW Approx. Gamma UTL with 90% Coverage 1486

#### BACKGROUND-SS-CADMIUM-UCL STATS

#### General Background Statistics for Data Sets with Non-Detects

# **User Selected Options**

From File Sheet1.wst

Full Precision OFF

Confidence Coefficient 95%

Coverage 90%

Different or Future K Values 1

Number of Bootstrap Operations 2000

SS\_Cadmium

#### **General Statistics**

Number of Valid Data 11

Number of Distinct Detected Data 1

Number of Detected Data 1

Number of Non-Detect Data 10

Warning: Only one distinct data value was detected! ProUCL (or any other software) should not be used on such a data set!

It is suggested to use alternative site specific values determined by the Project Team to estimate environmental parameters (e.g., EPC, BTV).

The data set for variable SS\_Cadmium was not processed!

### User Selected Options

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Coverage 90%

Different or Future K Values 1
Number of Bootstrap Operations 2000

#### SS\_Chromium

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 14

Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statist
naw Statistics	Log- i ransiorineu Statist

Minimum 0.9 Minimum -0.105 Maximum 92.3 Maximum 4.525 Second Largest 38.9 Second Largest 3.661 First Quartile 2.9 First Quartile 0.971 Median 1.569 Median 4.8 Third Quartile 9.1 Third Quartile 2.155 Mean 13.86 Mean 1.717 Geometric Mean 5.567 SD 1.32

SD 24.06 Coefficient of Variation 1.737

Skewness 2.879

### **Background Statistics**

#### Normal Distribution Test Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.569 Shapiro Wilk Test Statistic 0.934 Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

#### Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

### Assuming Normal Distribution Assuming Lognormal Distribution

95% UTL with 90% Coverage 63.62 95% UTL with 90% Coverage 85.4 95% UPL (t) 57.63 95% UPL (t) 61.48 90% Percentile (z) 44.7 90% Percentile (z) 30.23 95% Percentile (z) 53.44 95% Percentile (z) 48.85

95% Percentile (z) 53.44 95% Percentile (z) 48.85 99% Percentile (z) 69.84 99% Percentile (z) 120.1

# Gamma Distribution Test Data Distribution Test

k star 0.578 Data appear Lognormal at 5% Significance Level
Theta Star 23.96

MLE of Mean 13.86

MLE of Standard Deviation 18.22 nu star 17.35

A-D Test Statistic 1.04 Nonparametric Statistics

5% A-D Critical Value 0.781 90% Percentile 33.38
K-S Test Statistic 0.293 95% Percentile 54.92
5% K-S Critical Value 0.231 99% Percentile 84.82

#### Data not Gamma Distributed at 5% Significance Level

95% HW Approx. Gamma UTL with 90% Coverage 64.96

### Assuming Gamma Distribution 95% UTL with 90% Coverage 92.3

90% Percentile 36.34 95% Percentile Bootstrap UTL with 90% Coverage 92.3 95% Percentile 50.53 95% BCA Bootstrap UTL with 90% Coverage 92.3 95% Percentile 84.96 95% Chebyshev UPL 122.2

95% WH Approx. Gamma UPL 51.91 Upper Threshold Limit Based upon IQR 18.4

95% HW Approx. Gamma UPL 52.54 95% WH Approx. Gamma UTL with 90% Coverage 62.74

#### BACKGROUND-SS-COPPER-UCL STATS

#### General Background Statistics for Data Sets with Non-Detects

### User Selected Options

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Coverage 90%

Different or Future K Values 1
Number of Bootstrap Operations 2000

#### SS\_Copper

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 14

Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statistics

Minimum 0.92 Minimum -0.0834 Maximum 39.9 Maximum 3.686 Second Largest 16.6 Second Largest 2.809 First Quartile 3.75 First Quartile 1.315 Median 1.775 Median 5.9 Third Quartile 12.45 Third Quartile 2.517 Mean 9.248 Mean 1.83 Geometric Mean 6.234 SD 0.927

SD 9.692 Coefficient of Variation 1.048 Skewness 2.502

### **Background Statistics**

#### Normal Distribution Test Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.718 Shapiro Wilk Test Statistic 0.985
Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

#### Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

### Assuming Normal Distribution Assuming Lognormal Distribution

95% UTL with 90% Coverage 29.29 95% UTL with 90% Coverage 42.35 95% UTL with 90% Coverage 42.35 95% UPL (t) 26.88 95% UPL (t) 33.63 90% Percentile (z) 21.67 90% Percentile (z) 20.44 95% Percentile (z) 25.19 95% Percentile (z) 28.62 99% Percentile (z) 31.8 99% Percentile (z) 53.81

# Gamma Distribution Test Data Distribution Test

k star 1.173 Data appear Gamma Distributed at 5% Significance Level
Theta Star 7.881
MLE of Mean 9.248
MLE of Standard Deviation 8.537

nu star 35.2

A-D Test Statistic 0.335

#### Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution 95% UTL with 90% Coverage 39.9

 90% Percentile 20.47
 95% Percentile Bootstrap UTL with
 90% Coverage 39.9

 95% Percentile 26.19
 95% BCA Bootstrap UTL with
 90% Coverage 39.9

 99% Percentile 39.34
 95% UPL 39.9

 95% Chebyshev UPL 52.88

95% WH Approx. Gamma UPL 27.6 Upper Threshold Limit Based upon IQR 25.5 95% HW Approx. Gamma UPL 28.39

95% WH Approx. Gamma UTL with 90% Coverage 31.92 95% HW Approx. Gamma UTL with 90% Coverage 33.32

#### BACKGROUND-SS-LEAD-UCL STATS

#### General Background Statistics for Data Sets with Non-Detects

### User Selected Options

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Coverage 90%

Different or Future K Values 1 Number of Bootstrap Operations 2000

#### SS\_Lead

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 14 Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statistics

Minimum 4 Minimum 1.386 Maximum 48 Maximum 3.871 Second Largest 32.3 Second Largest 3.475 First Quartile 5.4 First Quartile 1.685 Median 2.95 Median 19.1 Third Quartile 25.3 Third Quartile 3.228 Mean 17.43 Mean 2.558 Geometric Mean 12.9 SD 0.84

SD 12.99 Coefficient of Variation 0.745

Skewness 0.857

### **Background Statistics**

#### **Normal Distribution Test Lognormal Distribution Test**

Shapiro Wilk Test Statistic 0.88 Shapiro Wilk Test Statistic 0.888 Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

#### **Assuming Normal Distribution Assuming Lognormal Distribution**

95% UTL with 90% Coverage 44.29 95% UTL with 90% Coverage 73.33 95% UPL (t) 41.06 95% UPL (t) 59.49 90% Percentile (z) 34.08 90% Percentile (z) 37.87 95% Percentile (z) 38.8 95% Percentile (z) 51.39 99% Percentile (z) 47.65 99% Percentile (z) 91.11

#### Data Distribution Test **Gamma Distribution Test**

nu star 44.85

k star 1.495 Data appear Gamma Distributed at 5% Significance Level Theta Star 11.66 MLE of Mean 17.43 MLE of Standard Deviation 14.25

A-D Test Statistic 0.714 Nonparametric Statistics

5% A-D Critical Value 0.749 90% Percentile 30 34 95% Percentile 37 01 K-S Test Statistic 0.21 5% K-S Critical Value 0.225 99% Percentile 45.8

Data appear Gamma Distributed at 5% Significance Level

#### **Assuming Gamma Distribution** 95% UTL with 90% Coverage 48

90% Percentile 36.34 95% Percentile Bootstrap UTL with 90% Coverage 48 95% Percentile 45.45 95% BCA Bootstrap UTL with 90% Coverage 41.72 99% Percentile 66.01 95% UPL 48 95% Chebyshev UPL 75.91

95% WH Approx. Gamma UPL 48.29 Upper Threshold Limit Based upon IQR 55.15

95% HW Approx. Gamma UPL 50.23

95% WH Approx. Gamma UTL with 90% Coverage 55.18 95% HW Approx. Gamma UTL with 90% Coverage 58.18

### User Selected Options

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Coverage 90%

Different or Future K Values 1
Number of Bootstrap Operations 2000

#### SS\_Manganese

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 15

Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statistics

Minimum 2.833 Minimum 17 Maximum 345 Maximum 5.844 Second Largest 219 Second Largest 5.389 First Quartile 34.05 First Quartile 3.527 Median 93.4 Median 4.537 Third Quartile 139 Third Quartile 4.934 Mean 107.5 Mean 4.325 Geometric Mean 75.55 SD 0.916

SD 90.39 Coefficient of Variation 0.841 Skewness 1.403

# **Background Statistics**

#### Normal Distribution Test Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.871 Shapiro Wilk Test Statistic 0.959
Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

#### Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

### Assuming Normal Distribution Assuming Lognormal Distribution

95% UTL with 90% Coverage 294.4 95% UTL with 90% Coverage 502.3 95% UPL (t) 271.9 95% UPL (t) 399.9 90% Percentile (z) 223.3 90% Percentile (z) 244.4 95% Percentile (z) 256.1 95% Percentile (z) 340.9 99% Percentile (z) 317.7 99% Percentile (z) 636.4

### Gamma Distribution Test Data Distribution Test

k star 1.297 **Data appear Gamma Distributed at 5% Significance Level**Theta Star 82.88
MLE of Mean 107.5

MLE of Standard Deviation 94.37 nu star 38.9

A-D Test Statistic 0.221 Nonparametric Statistics

5% A-D Critical Value 0.753 90% Percentile 207.4
K-S Test Statistic 0.146 95% Percentile 256.8
5% K-S Critical Value 0.225 99% Percentile 327.4

#### Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution 95% UTL with 90% Coverage 345

 90% Percentile 232.1
 95% Percentile Bootstrap UTL with
 90% Coverage 345

 95% Percentile 294.1
 95% BCA Bootstrap UTL with
 90% Coverage 345

 99% Percentile 435.5
 95% UPL 345

 95% Chebyshev UPL 514.4

95% WH Approx. Gamma UPL 312.9 Upper Threshold Limit Based upon IQR 296.4

95% HW Approx. Gamma UPL 326.5

95% WH Approx. Gamma UTL with 90% Coverage 360.1 95% HW Approx. Gamma UTL with 90% Coverage 381.4

### User Selected Options

From File Sheet1.wst
Full Precision OFF
Confidence Coefficient 95%
Coverage 90%

Different or Future K Values 1
Number of Bootstrap Operations 2000

#### SS\_Mercury

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 11

Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statistics

Minimum 0.0044 Minimum -5.426 Maximum 0.025 Maximum -3.689 Second Largest 0.015 Second Largest -4.2 First Quartile 0.0078 First Quartile -4.868 Median -4.51 Median 0.011 Third Quartile 0.012 Third Quartile -4.423 Mean 0.011 Mean -4.594 Geometric Mean 0.0101 SD 0.426

SD 0.00492 Coefficient of Variation 0.447

Skewness 1.547

### **Background Statistics**

#### Normal Distribution Test Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.865 Shapiro Wilk Test Statistic 0.957
Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

#### Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

### Assuming Normal Distribution Assuming Lognormal Distribution

95% UTL with 90% Coverage 0.0212 95% UTL with 90% Coverage 0.0244
95% UPL (t) 0.02 95% UPL (t) 0.022
90% Percentile (z) 0.0173 90% Percentile (z) 0.0191
95% Percentile (z) 0.025 99% Percentile (z) 0.0273

#### Gamma Distribution Test Data Distribution Test

k star 4.888 Data appear Gamma Distributed at 5% Significance Level
Theta Star 0.00225
MLE of Mean 0.011

MLE of Standard Deviation 0.00498 nu star 146.6

A-D Test Statistic 0.4 Nonparametric Statistics

 5% A-D Critical Value 0.738
 90% Percentile 0.0146

 K-S Test Statistic 0.163
 95% Percentile 0.018

 5% K-S Critical Value 0.222
 99% Percentile 0.0236

#### Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution 95% UTL with 90% Coverage 0.025

 90% Percentile 0.0177
 95% Percentile Bootstrap UTL with
 90% Coverage 0.025

 95% Percentile 0.0203
 95% BCA Bootstrap UTL with
 90% Coverage 0.021

 99% Percentile 0.0257
 95% UPL 0.025

 95% Chebyshev UPL 0.0332

95% WH Approx. Gamma UPL 0.0208 Upper Threshold Limit Based upon IQR 0.0183

95% HW Approx. Gamma UPL 0.021

95% WH Approx. Gamma UTL with 90% Coverage 0.0226 95% HW Approx. Gamma UTL with 90% Coverage 0.023

### User Selected Options

 From File
 Sheet1.wst

 Full Precision
 OFF

 Confidence Coefficient
 95%

 Coverage
 90%

 Different or Future K Values
 1

Different or Future K Values 1

Number of Bootstrap Operations 2000

#### SS\_Vanadium

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 15

Tolerance Factor 2.068

Raw Statistics	Log-Transformed Statistics
----------------	----------------------------

Minimum 0.93 Minimum -0.0726 Maximum 23.7 Maximum 3.165 Second Largest 13.9 Second Largest 2.632 First Quartile 2.85 First Quartile 1.047 Median 1.758 Median 5.8 Third Quartile 7.25 Third Quartile 1.977 Mean 6.595 Mean 1.56 Geometric Mean 4.758 SD 0.873

SD 5.787 Coefficient of Variation 0.877 Skewness 2.06

#### **Background Statistics**

#### Normal Distribution Test Lognormal Distribution Test

Shapiro Wilk Test Statistic 0.787 Shapiro Wilk Test Statistic 0.958
Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

#### Data not Normal at 5% Significance Level Data appear Lognormal at 5% Significance Level

### Assuming Normal Distribution Assuming Lognormal Distribution

95% UTL with 90% Coverage 18.56 95% UTL with 90% Coverage 28.95
95% UPL (t) 17.12 95% UPL (t) 23.29
90% Percentile (z) 14.01 90% Percentile (z) 14.57
95% Percentile (z) 16.11 95% Percentile (z) 20.01
99% Percentile (z) 20.06 99% Percentile (z) 36.27

# Gamma Distribution Test Data Distribution Test

k star 1.387 **Data appear Gamma Distributed at 5% Significance Level**Theta Star 4.754
MLE of Mean 6.595

MLE of Standard Deviation 5.599 nu star 41.62

A-D Test Statistic 0.349 Nonparametric Statistics

 5% A-D Critical Value 0.751
 90% Percentile 11.78

 K-S Test Statistic 0.136
 95% Percentile 16.84

 5% K-S Critical Value 0.225
 99% Percentile 22.33

#### Data appear Gamma Distributed at 5% Significance Level

#### Assuming Gamma Distribution 95% UTL with 90% Coverage 23.7

90% Percentile 14.01 95% Percentile Bootstrap UTL with 90% Coverage 23.7 95% Percentile 17.64 95% BCA Bootstrap UTL with 90% Coverage 19.78 99% Percentile 25.87 95% UPL 23.7 95% Chebyshev UPL 32.65

95% WH Approx. Gamma UPL 18.62 Upper Threshold Limit Based upon IQR 13.85

95% HW Approx. Gamma UPL 19.31

95% WH Approx. Gamma UTL with 90% Coverage 21.35 95% HW Approx. Gamma UTL with 90% Coverage 22.44

### User Selected Options

From File Sheet1.wst Full Precision OFF Confidence Coefficient 95% Coverage 90%

Different or Future K Values 1 Number of Bootstrap Operations 2000

SS\_Zinc

#### **General Statistics**

Total Number of Observations 15 Number of Distinct Observations 15 Tolerance Factor 2.068

#### **Raw Statistics** Log-Transformed Statistics

Minimum 2.219 Minimum 9.2 Maximum 3630 Maximum 8.197 Second Largest 203 Second Largest 5.313 First Quartile 18.45 First Quartile 2.915 Median 4.004 Median 54.8 Third Quartile 86.25 Third Quartile 4.442 Mean 299 Mean 4.062 Geometric Mean 58.08 SD 1.434

SD 922.9 Coefficient of Variation 3.087

Skewness 3.853

#### **Background Statistics**

#### **Normal Distribution Test Lognormal Distribution Test**

Shapiro Wilk Test Statistic 0.328 Shapiro Wilk Test Statistic 0.851 Shapiro Wilk Critical Value 0.881 Shapiro Wilk Critical Value 0.881

#### Data not Normal at 5% Significance Level Data not Lognormal at 5% Significance Level

#### **Assuming Normal Distribution Assuming Lognormal Distribution**

95% UTL with 90% Coverage 2208 95% UTL with 90% Coverage 1127 95% UPL (t) 1978 95% UPL (t) 788.7 90% Percentile (z) 1482 90% Percentile (z) 364.9 95% Percentile (z) 1817 95% Percentile (z) 614.4 99% Percentile (z) 2446 99% Percentile (z) 1633

#### Data Distribution Test **Gamma Distribution Test**

k star 0.366 Data do not follow a Discernable Distribution (0.05) Theta Star 817.9

MLE of Mean 299 MLE of Standard Deviation 494.5 nu star 10.97

> A-D Test Statistic 2.443 Nonparametric Statistics

5% A-D Critical Value 0.814 90% Percentile 169 K-S Test Statistic 0.352 95% Percentile 1231 5% K-S Critical Value 0.237 99% Percentile 3150

#### Data not Gamma Distributed at 5% Significance Level

#### **Assuming Gamma Distribution** 95% UTL with 90% Coverage 3630

90% Percentile 857.5 95% Percentile Bootstrap UTL with 90% Coverage 3630 95% Percentile 1281 95% BCA Bootstrap UTL with 90% Coverage 3630 99% Percentile 2357 95% UPL 3630 95% Chebyshev UPL 4454

95% WH Approx. Gamma UPL 1078 Upper Threshold Limit Based upon IQR 188 95% HW Approx. Gamma UPL 973.8

95% WH Approx. Gamma UTL with 90% Coverage 1348 95% HW Approx. Gamma UTL with 90% Coverage 1249